

## 1.5. Linear Elasticity, Plasticity, Compatibility, and Field Equations

*"THE BLADES DO NOT MESH.*

*How is the geometric structure at one point in space-time related to that at a neighboring point? A geometrical description of the electromagnetic field has to answer this question. It therefore appeared useful to us to raise the issue, what happens when one moves in the local two dimensional surface, or tangent plane, of blade A to neighboring points where blade A is tilted at slightly different orientations. Will one arrive in this way at a well defined two dimensional surface,*

$$x^\mu = x_A^\mu(u, v) ? \quad (58)$$

*Or will the pattern of blades lead to structures like those in a spiral dislocation in a crystal, so that one can get from one point to any other point by moving about on blades A via a suitably selected route? In this case no surface of type (58) will exist." From Misner and Wheeler (1957).<sup>[12]</sup>*

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[12]: See de Wit (1960) and Golebiewska-Lasota (1979) for discussion of the similarities between electromagnetism and dislocation theory. *Blades* are discussed by Schouten (1954) and Eringen (1971).

Components,  $\varepsilon_{ab}$ , of the *linear elastic strain tensor*,  $\boldsymbol{\varepsilon}$ ,

$$\boldsymbol{\varepsilon} \equiv \varepsilon_{ab} \vec{dx}^a \otimes \vec{dx}^b,$$

are

$$\varepsilon_{ab} \equiv \frac{1}{2}(\partial u_b / \partial x^a + \partial u_a / \partial x^b) \equiv \frac{1}{2}(\partial_a u_b + \partial_b u_a) \equiv u_{(b,a)}.$$

The equivalent matrix representation is

$$\varepsilon_{ab} \equiv \begin{vmatrix} \varepsilon_{xx} & \varepsilon_{yx} & \varepsilon_{zx} \\ \varepsilon_{xy} & \varepsilon_{yy} & \varepsilon_{zy} \\ \varepsilon_{xz} & \varepsilon_{yz} & \varepsilon_{zz} \end{vmatrix}.$$

Components,  $\omega_{ab}$ , of the *linear elastic rotation tensor*,  $\boldsymbol{\omega}$ ,

$$\boldsymbol{\omega} \equiv \frac{1}{2} \omega_{ab} \vec{dx}^a \wedge \vec{dx}^b \equiv \omega_{[ab]} \vec{dx}^a \wedge \vec{dx}^b,$$

are

$$-\omega_{ba} = \omega_{ab} \equiv \frac{1}{2}(\partial_a u_b - \partial_b u_a) \equiv u_{[b,a]}.$$

The equivalent matrix representation is

$$\omega_{ab} \equiv \begin{vmatrix} 0 & \omega_{yx} & \omega_{zx} \\ \omega_{xy} & 0 & \omega_{zy} \\ \omega_{xz} & \omega_{yz} & 0 \end{vmatrix}.$$

Thus, since  ${}^b\mathbf{u} = u_b \vec{dx}^b$ ,  $\boldsymbol{\omega} = \vec{d}{}^b\mathbf{u} = \partial_a u_b \vec{dx}^a \wedge \vec{dx}^b = \frac{1}{2}(\partial_a u_b - \partial_b u_a) \vec{dx}^a \wedge \vec{dx}^b$ . If  $\boldsymbol{\omega} = \mathbf{0}$ , then there is some function  $f$  such that  $\vec{d}f = u_a \vec{dx}^a$ ,  $u_a = \partial f / \partial x^a$  (Flanders 1989). The dual

of  $\omega$ ,  ${}^*\omega$ , is the 1-form  $\tilde{\omega} \equiv {}^*\omega$  given by  $\tilde{\omega} \equiv \frac{1}{2}\epsilon_{abc}\omega^{bc}\vec{dx}^a$ , with components  $\tilde{\omega}_a = \frac{1}{2}\epsilon_{abc}\omega^{bc}$ , where  $\omega^{bc} = \omega_{bc}$  only because the  $x^a$  coordinates are orthonormal. This 1-form  $\tilde{\omega} \equiv {}^*\omega$  always has the same components as  $\omega$ :  $\tilde{\omega} = \omega_y\vec{dx} + \omega_x\vec{dy} + \omega_z\vec{dz}$ .

The *linear elastic distortion tensor* is

$$\gamma \equiv \epsilon + \omega,$$

and its components are just, for example,

$$\gamma_{ab} \equiv \partial u_b / \partial x^a,$$

when the differentiation is allowable.

Since  $\epsilon$  is symmetric,  $\epsilon_{ab} = \frac{1}{2}(\partial u_b / \partial x^a + \partial u_a / \partial x^b)$  is a system of six partial differential equations,  $\{\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}, \epsilon_{xy}, \epsilon_{yz}, \epsilon_{xz}\}$  with only three unknowns,  $\{u_x, u_y, u_z\}$ ; so it is *overdetermined* (Malvern 1969). The integrability conditions are *St-Venant's compatibility equations*, written after Eshelby (1956), as follows: The vector,  $\vec{\omega}$ , corresponding to the 1-form  $\tilde{\omega} \equiv {}^*\omega \equiv \frac{1}{2}\epsilon_{abc}\omega^{bc}\vec{dx}^a$  is  $\vec{\omega} \equiv \frac{1}{2}\epsilon^{abc}\omega_{bc}\vec{d}_a \equiv \frac{1}{2}\epsilon^{abc}\omega_{bc}\vec{i}_a$ ,  $\vec{\omega}^a \equiv \frac{1}{2}\epsilon^{abc}\omega_{bc}$ . Components of  $\vec{\omega}$  and  $\vec{\omega}$  are identical in an orthonormal frame only. The relationships  $\epsilon_{ab} = u_{(b,a)}$  and  $\omega_{ab} = u_{[b,a]}$  imply that  $\omega_{ab,c} = \epsilon_{cb,a} - \epsilon_{ca,b}$ , or since  $\vec{\omega}^d = \frac{1}{2}\epsilon^{dab}\omega_{ab}$ , the following instead:

$$\begin{aligned} \vec{\omega}_{,c}^d &= \frac{1}{2}\epsilon^{dab}\omega_{ab,c} = \frac{1}{2}\epsilon^{dab}(\epsilon_{cb,a} - \epsilon_{ca,b}), \\ &= \frac{1}{2}\epsilon^{dab}\epsilon_{cb,a} - \frac{1}{2}\epsilon^{dab}\epsilon_{cb,a}, \text{ (index exchange on second term)} \\ &= \frac{1}{2}(\epsilon^{dab} - \epsilon^{dba})\epsilon_{cb,a}, \\ &= \epsilon^{dab}\epsilon_{cb,a}, (\epsilon^{dba} = -\epsilon^{dab}) \\ &\equiv [\epsilon \times \vec{\nabla}]_c^d. \quad ([\nabla \times]^a = \epsilon^{abc}\partial(...)/\partial x^b; \text{ "slot" for 'c' index.}) \end{aligned}$$

Here, the arrow over the gradient operator indicates that it is operating on the right-most index. Now  $\vec{\omega}_{,c}^d = \epsilon^{dab} \varepsilon_{cb,a}$  are components of a "vector-valued" 1-form<sup>[13]</sup>  $\vec{\omega}_{,c}^d \vec{dx}^c$ , which could be referred to "abstractly" as  ${}^b\nabla\vec{\omega}$ . If  $\vec{\omega}_{,c}^d \vec{dx}^c$  is in fact such a "gradient," then

$$\oint {}^b\nabla\vec{\omega} = \oint \vec{\omega}_{,c}^d \vec{dx}^c = \oint \epsilon^{dab} \varepsilon_{cb,a} dx^c = 0,$$

or

$$\oint dI \bullet \boldsymbol{\epsilon} \times \vec{\nabla} = 0.$$

Equivalently, the curl of the integrand vanishes:

$$\vec{\nabla} \times \boldsymbol{\epsilon} \times \vec{\nabla} = 0,$$

or

$$\epsilon^{efc} \epsilon^{dab} \varepsilon_{cb,af} = 0.$$

Rearranging the indices and multiplying by  $-1$ ,

$$-\epsilon^{ace} \epsilon^{bdf} \varepsilon_{cf,dc} \equiv N^{ab}$$

are components of the *incompatibility tensor* (Malvern 1969)

$$\mathbf{N} \equiv N^{ab} \mathbf{i}_a \otimes \mathbf{i}_b \equiv -\epsilon^{ace} \epsilon^{bdf} \varepsilon_{cf,dc} \mathbf{i}_a \otimes \mathbf{i}_b \equiv -\vec{\nabla} \times \boldsymbol{\epsilon} \times \vec{\nabla}.$$

[13]: Terminology from Misner *et al.* (1973).

When  $\mathbf{N}(\boldsymbol{\varepsilon}) = \mathbf{0}$  in a simply-connected elastic body then  $\mathbf{u}$  and  $\boldsymbol{\varepsilon}$  can be defined for every point of the body,  $\vec{d}^b \mathbf{u}$  is exact, and  $\boldsymbol{\varepsilon}$  has components  $\varepsilon_{ab} \equiv \frac{1}{2}(\partial u_a / \partial x_b + \partial u_b / \partial x_a)$  in the linear approximation. The components of  $\mathbf{N}$  can be rearranged to read

$$\varepsilon_{ab,cd} - \varepsilon_{ac,bd} = \varepsilon_{db,ca} - \varepsilon_{dc,ba},$$

which are the *integrability conditions* for the strain  $\boldsymbol{\varepsilon}$ . The incompatibility tensor  $\mathbf{N}$  is symmetric (Malvern 1969). The six relationships from it are not independent conditions since even if  $\mathbf{N} \neq \mathbf{0}$ ,  $\mathbf{N}$  satisfies the *Bianchi identities* (Malvern 1969),

$$\nabla \cdot \mathbf{N} = 0,$$

because  $\mathbf{N}$  is defined by a curl.

**Conservation laws expressing topological stability are called "Bianchi identities." In elasticity the topological objects are dislocations and disclinations. These conservation laws constrain the motion of such defects and the media in which they reside** (Rivier 1987).

"If the displacement functions are included explicitly as unknowns in formulating the elasticity boundary-value problem, then the compatibility equations are not needed" (Malvern 1969). This is not the case, however, if points in the material are represented parametrically. Since the response of a crystal to either external or internal loads is anisotropic, it is

reasonable to expect some sort of parametric treatment to this problem. Even if anisotropy is addressed very simply, as it is here, by saying that the Burgers vector is in the close-packed direction of the lattice.

The "standard" definition of the Burgers vector  $\mathbf{b} = \oint (\partial \mathbf{u} / \partial s) ds$  can be reexpressed as  $b^a = \oint_C \vec{d}u^a$ , where  $C$  is a closed path that links the dislocation axis with a right-hand screw sense and  $\mathbf{b} \equiv b^a \mathbf{i}_a$  (de Wit 1960). Since the integral is by definition non-vanishing  $\vec{d}u^a \equiv \gamma_{b^a} \vec{d}x^b$  is a Pfaffian (equivalently: not a perfect differential, an inexact 1-form), with the coefficients  $\gamma_{b^a}$  being the distortions. If  $\vec{d}u^a$  is exact, then  $\vec{d}u^a = (\partial u^a / \partial x^b) \vec{d}x^b \equiv \gamma_{b^a} \vec{d}x^b$ , and the distortions  $\gamma_{b^a}$  are the "gradients"  $\partial u^a / \partial x^b$ , so  $\oint_C \vec{d}u^a = \oint_C \gamma_{b^a} \vec{d}x^b = 0$ , *i.e.* there is no dislocation line passing through  $C$ . When there are dislocations in some region, then  $\vec{d}u^a$  is inexact;  $\mathbf{u}$  may be locally continuous but it diverges, and there is a "source." Components for the strain tensor are written as

$$\varepsilon_{ab} = \frac{1}{2}(\gamma_{ba} + \gamma_{ab}) = \gamma_{(ba)}$$

with the completely covariant form of the distortions. This agrees with the former definition of the strain when  $\vec{d}u^a$  is exact,  $\vec{d}u^a = (\partial u^a / \partial x^b) \vec{d}x^b \equiv \gamma_{b^a} \vec{d}x^b$ ; otherwise it can be taken as a more general definition.

The integral for the Burgers vector can be converted from line to surface with Stokes' theorem,  $\oint_C \boldsymbol{\alpha} = \int_S \vec{d}\boldsymbol{\alpha}$ , where  $S$  is a surface that bounds the closed curve  $C$ , and  $\boldsymbol{\alpha} = \alpha_a \vec{d}x^a$  is a 1-form:

$$\oint_C \vec{d}u^a = \int_S \vec{d}^2 u^a,$$

where

$$\begin{aligned}
\vec{\mathbf{d}}^2 u^a &\equiv \vec{\mathbf{d}} \vec{\mathbf{d}} u^a \equiv \vec{\mathbf{d}}(\gamma_b^a \vec{\mathbf{d}} x^b) = (\partial_c \gamma_b^a / \partial x^c) \vec{\mathbf{d}} x^c \wedge \vec{\mathbf{d}} x^b, \\
&\equiv \partial_c \gamma_b^a \vec{\mathbf{d}} x^c \wedge \vec{\mathbf{d}} x^b, \\
&\equiv \tfrac{1}{2} (\partial_c \gamma_b^a - \partial_b \gamma_c^a) \vec{\mathbf{d}} x^c \wedge \vec{\mathbf{d}} x^b, \\
&\equiv \tfrac{1}{2} T_{cb}^a \vec{\mathbf{d}} x^c \wedge \vec{\mathbf{d}} x^b.
\end{aligned}$$

Here,  $T_{cb}^a \equiv \partial_c \gamma_b^a - \partial_b \gamma_c^a$  are components of the torsion tensor, which all vanish identically when the Poincaré Lemma,  $\vec{\mathbf{d}}^2 u^a = \mathbf{0}$ , holds,  $\vec{\mathbf{d}}^2 u^a \equiv \vec{\mathbf{d}}(\gamma_b^a \vec{\mathbf{d}} x^b) = \mathbf{0}$  if  $\gamma_b^a \equiv \partial u^a / \partial x^b$ ; also, the "differential" surface area for  $\mathbf{S}$  is  $\vec{\mathbf{d}} x^c \wedge \vec{\mathbf{d}} x^b$ . Note that

$$\vec{\mathbf{d}}^2 u^a \equiv \vec{\mathbf{d}}(\gamma_b^a \vec{\mathbf{d}} x^b) \equiv \vec{\mathbf{d}} \tilde{\boldsymbol{\gamma}}^a \equiv \text{rot } \tilde{\boldsymbol{\gamma}}^a \equiv \tfrac{1}{2} T_{cb}^a \vec{\mathbf{d}} x^c \wedge \vec{\mathbf{d}} x^b, \quad \text{□}$$

where  $\tilde{\boldsymbol{\gamma}}^a \equiv \gamma_b^a \vec{\mathbf{d}} x^b$  are the *distortion 1-forms* (Edelen 1979), the superscript denoting a specific 1-form, not any particular components. de Wit (1960), on the other hand, uses the dual "differential" surface area,  $\tfrac{1}{2} G_{dc} \boldsymbol{\epsilon}^{ccb} \vec{\mathbf{d}} x^d$  for  $\mathbf{S}$ :

$$\int_S \vec{\mathbf{d}}^2 u^a = \int_S \partial_c \gamma_b^a \vec{\mathbf{d}} x^c \wedge \vec{\mathbf{d}} x^b = \int_S G_{dc} \boldsymbol{\epsilon}^{ccb} \partial_c \gamma_b^a \vec{\mathbf{d}} x^d.$$

The object  $G_{dc} \boldsymbol{\epsilon}^{ccb} \partial_c \gamma_b^a \vec{\mathbf{d}} x^d = \boldsymbol{\epsilon}^{ccb} \partial_c \gamma_b^a (G_{dc} \vec{\mathbf{d}} x^d) = \boldsymbol{\epsilon}^{ccb} \partial_c \gamma_b^a \mathbf{i}_e = \boldsymbol{\epsilon}^{dcb} \partial_c \gamma_b^a \mathbf{i}_d$ , where  $\mathbf{i}_e = G_{dc} \vec{\mathbf{d}} x^d$ , suggests that the *dislocation density tensor* is

$$\boldsymbol{\rho} \equiv \rho^{da} \mathbf{i}_d \otimes \mathbf{i}_a \equiv \boldsymbol{\epsilon}^{dcb} \partial_c \gamma_b^a \mathbf{i}_d \otimes \mathbf{i}_a \equiv \nabla \times \boldsymbol{\gamma}. \quad \text{□}$$

Also,

$$\boldsymbol{\epsilon}^{dcb} \partial_c \gamma_b^a = \frac{1}{2} \boldsymbol{\epsilon}^{dcb} (\partial_c \gamma_b^a - \partial_b \gamma_c^a) = \frac{1}{2} \boldsymbol{\epsilon}^{dcb} T_{cb}^a;$$

therefore

$$\rho^{da} = \frac{1}{2} \boldsymbol{\epsilon}^{dcb} T_{cb}^a. \quad \text{□}$$

Note that  $\boldsymbol{\epsilon}_{def} \rho^{da} \equiv \boldsymbol{\epsilon}_{def} \boldsymbol{\epsilon}^{dcb} \partial_c \gamma_b^a \equiv (\delta_e^c \delta_f^b - \delta_f^c \delta_e^b) \partial_c \gamma_b^a = \partial_c \gamma_f^a - \partial_f \gamma_c^a \equiv T_{ef}^a$ ; thus,

$$T_{bc}^a = \boldsymbol{\epsilon}_{dbc} \rho^{da}. \quad \text{□}$$

The dislocation density and torsion tensors are "dual" objects.

Components  $\rho^{af}$  of the dislocation density tensor  $\boldsymbol{\rho} = \rho^{af} \mathbf{i}_a \otimes \mathbf{i}_f$  give the *field equations*,  
 $\rho^{af} = \boldsymbol{\epsilon}^{acc} \partial_c \gamma_e^f$  (de Wit 1960): dislocations ( $\boldsymbol{\rho}$ ) are the source of the (three) fields  $\tilde{\boldsymbol{\gamma}}^f \equiv \gamma_e^f \vec{dx}^e$  (with nine coefficients  $\gamma_e^f$ ). Now let the operator  $\boldsymbol{\epsilon}^{bdf} \partial_d (\times \vec{\nabla})$  act on  $(\rho^{af} = \boldsymbol{\epsilon}^{acc} \partial_c \gamma_e^f)^b$   
 $= \rho^a_f = \boldsymbol{\epsilon}^{acc} \partial_c \gamma_{ef}$ :

$$\boldsymbol{\epsilon}^{bdf} \partial_d \rho^a_f = \boldsymbol{\epsilon}^{acc} \boldsymbol{\epsilon}^{bdf} \partial_c \partial_d \gamma_{ef} \equiv \boldsymbol{\epsilon}^{acc} \boldsymbol{\epsilon}^{bdf} \gamma_{ef,dc}.$$

The following "index gymnastics" relate this expression to the incompatibility tensor  $\mathbf{N}$ :

$$\begin{aligned}
\frac{1}{2}(\boldsymbol{\epsilon}^{bdf}\partial_d\rho_f^a + \boldsymbol{\epsilon}^{adf}\partial_d\rho_f^b) &= \frac{1}{2}(\boldsymbol{\epsilon}^{ace}\boldsymbol{\epsilon}^{bdf}\gamma_{ef,dc} + \boldsymbol{\epsilon}^{bce}\boldsymbol{\epsilon}^{adf}\gamma_{ef,dc}), \text{ ("symmetrizing" on a,b)} \\
&= \frac{1}{2}(\boldsymbol{\epsilon}^{ace}\boldsymbol{\epsilon}^{bdf}\gamma_{cf,dc} + \boldsymbol{\epsilon}^{bcf}\boldsymbol{\epsilon}^{adc}\gamma_{fc,dc}), \text{ (exchange of e,f in second term)} \\
&= \frac{1}{2}(\boldsymbol{\epsilon}^{ace}\boldsymbol{\epsilon}^{bdf}\gamma_{ef,dc} + \boldsymbol{\epsilon}^{bdf}\boldsymbol{\epsilon}^{ace}\gamma_{fe,cd}), \text{ (exchange of c,d in second term)} \\
&= \frac{1}{2}(\boldsymbol{\epsilon}^{ace}\boldsymbol{\epsilon}^{bdf}\gamma_{ef,dc} + \boldsymbol{\epsilon}^{bdf}\boldsymbol{\epsilon}^{ace}\gamma_{fe,dc}), \text{ (partial differentiation commutes)<sup>[14]</sup>} \\
&= \frac{1}{2}\boldsymbol{\epsilon}^{ace}\boldsymbol{\epsilon}^{bdf}(\gamma_{ef,dc} + \gamma_{fe,dc}), \\
&= \boldsymbol{\epsilon}^{ace}\boldsymbol{\epsilon}^{bdf}\varepsilon_{ef,dc}, \quad (\varepsilon_{ef} \equiv \frac{1}{2}[\gamma_{fe} + \gamma_{ef}]) \\
&\equiv -N^{ab}.
\end{aligned}$$

The object  $\frac{1}{2}(\boldsymbol{\epsilon}^{bdf}\partial_d\rho_f^a + \boldsymbol{\epsilon}^{adf}\partial_d\rho_f^b)$  is "symmetrized" on the a,b indices:  $\frac{1}{2}(\boldsymbol{\epsilon}^{bdf}\partial_d\rho_f^a + \boldsymbol{\epsilon}^{adf}\partial_d\rho_f^b)$   
 $\equiv \boldsymbol{\epsilon}^{(b|df|\partial_d\rho_f^a)}$  (de Wit 1960, Nabarro 1967); the vertical bars mean that the enclosed indices are excluded from "symmetrization." Summarizing,

$$N^{ab} \equiv -\boldsymbol{\epsilon}^{ace}\boldsymbol{\epsilon}^{bdf}\varepsilon_{ef,dc} = -\boldsymbol{\epsilon}^{(b|df|\partial_d\rho_f^a)} \equiv -\frac{1}{2}(\boldsymbol{\epsilon}^{bdf}\partial_d\rho_f^a + \boldsymbol{\epsilon}^{adf}\partial_d\rho_f^b), \quad \text{[14]}$$

or symbolically,

$$\mathbf{N} \equiv -\vec{\nabla} \times \boldsymbol{\varepsilon} \times \vec{\nabla} = -{}^{symm}(\nabla \times \mathbf{p});$$

dislocations are a source of incompatibility, if  $\mathbf{p} = \mathbf{0}$ , then  $\mathbf{N} = \mathbf{0}$ . Since  $\mathbf{N}(\mathbf{p})$  is defined by a curl,  $\nabla \cdot \mathbf{N} = 0$  is an identity.

[14]: Partial differentiation commutes in a holonomic coordinate system such as  $\{x^a\}$

(Misner *et al.* 1973).

The dislocation density tensor  $\rho \equiv \nabla \times \gamma$  is defined by a curl too, therefore

$$\nabla \cdot \rho = 0$$

is an identity which means that dislocations do not end in a lattice free of disclinations: dislocation lines form either closed loops or terminate at the surface of the lattice. If there are no disclinations in the lattice then there is no "source" for dislocation lines.

**Field equations have a purely local character, relating conditions at one point to conditions at points an infinitesimal distance away. They tell nothing about the topology of space in the large** (Misner and Wheeler 1957).

**Generating the "Source:"** How is the "source" of the elastic displacement field associated with a dislocation described mathematically? A dislocation is of *Burgers' type* if it produces a multiple-valued displacement field such that the magnitude of  $\mathbf{u}$  increases by  $\|\mathbf{b}\|$  for every circuit taken around the dislocation line. For a dislocation loop that subtends a solid angle  $O$  at point  $\rho$ , *Burgers multivalued displacement function* is (de Wit 1960, Nabarro 1967, Landau and Lifshitz 1986)

$$-\mathbf{u}(\rho) = O \frac{\mathbf{b}}{4\pi} + \frac{\mathbf{b}}{4\pi} \times \oint_L \frac{d\xi}{r} + \frac{\lambda + G}{4\pi(\lambda + 2G)} \nabla \oint_L \frac{\mathbf{b} \times (\rho - \rho_0)}{r} \cdot d\xi.$$

Here,  $\lambda$  is Lamé's constant,  $G$  is the shear modulus,  $d\xi$  is a differential segment of the dislocation line at a point  $\rho$  on the loop  $L$ , and  $r \equiv \|\rho - \rho_0\|$ . The last two terms of this expression are single-valued functions of position, but the first term changes by  $4\pi$  when  $O$  links  $C$ :  $\oint_C d^a u = -(b/4\pi) \oint_C dO = b$ . I have used the superscript ' $a$ ' for the displacement field " $u$ " to indicate that it is a "dislocation displacement field"; it generates, or is the source of an elastic displacement field  $u$ .

Away from the dislocation core the displacements  $u$  are well defined and vary continuously in the body (Friedel 1979), and therefore the elastic strain tensor  $\epsilon$  is compatible,  $N(\epsilon) = 0$ , in these regions. The compatibility equation for the elastic strain is, on the other hand, not satisfied along the dislocation line,  $N(\epsilon_{(\rho_0)}) \neq 0$ . The dislocation core can be considered as a line of "singularities" in an "elastic field" (Kosevich 1979): For example, if  $n$  is a unit vector normal to the surface containing the dislocation loop, then

$${}^a\epsilon \equiv \frac{1}{2}(n \otimes b + b \otimes n)\delta(n),$$

is the *dislocation strain tensor*,  $n$  being a coordinate along the direction  $n$  with  $\delta(n)$  denoting the Dirac delta function (Kosevich 1979). The distortion, torsion, and dislocation density tensors can all be written in a similar fashion, e.g. " $\gamma$ " for the distortion. The dislocation distortion " $\gamma$ " can be viewed as a "potential"<sup>[15]</sup> for the dislocation density tensor, " $\rho$ ",

[15]: "Any vector  $v$  that vanishes at infinity can be decomposed into a "gradient" and a "curl,"  $v = \nabla f + \nabla \times {}^b p$ " (de Wit 1960). Here,  $f$  is some function, called the *potential*, and  $p$  is a vector called the *vector potential*.

${}^d\boldsymbol{\rho} \equiv \nabla \times {}^d\boldsymbol{\gamma}$ ; similarly  $\mathbf{N}({}^d\boldsymbol{\epsilon}) = -{}^{symm}(\nabla \times {}^d\boldsymbol{\rho})$  (Nabarro 1967).

The compatibility equation for the *internal strain*,  ${}^I\boldsymbol{\epsilon}$ , defined as the sum of the elastic and dislocation strains,  ${}^I\boldsymbol{\epsilon} \equiv \boldsymbol{\epsilon} + {}^d\boldsymbol{\epsilon}$ , is, in the linear approximation satisfied (Nabarro 1967, de Wit 1981):

$$\mathbf{N}({}^I\boldsymbol{\epsilon}) = \mathbf{N}(\boldsymbol{\epsilon}) + \mathbf{N}({}^d\boldsymbol{\epsilon}) = \mathbf{0}, \quad [16]$$

or since  $\mathbf{N}({}^e\boldsymbol{\epsilon}) = -\vec{\nabla} \times {}^e\boldsymbol{\epsilon} \times \hat{\vec{\nabla}} = -{}^{symm}(\nabla \times {}^e\boldsymbol{\rho})$ ,

$$\vec{\nabla} \times \boldsymbol{\epsilon} \times \hat{\vec{\nabla}} = -\vec{\nabla} \times {}^d\boldsymbol{\epsilon} \times \hat{\vec{\nabla}} = -{}^{symm}(\nabla \times {}^d\boldsymbol{\rho}).$$

This implies that

$$\nabla \times \boldsymbol{\rho} = -\nabla \times {}^d\boldsymbol{\rho}. \quad [17]$$

Thus, if defects are present with a distribution given by some function  $\mathbf{N}({}^d\boldsymbol{\epsilon}) = -{}^{symm}(\nabla \times {}^d\boldsymbol{\rho})$ , then elastic strain  $\boldsymbol{\epsilon}$  is produced according to  $\mathbf{N}(\boldsymbol{\epsilon}) = -\mathbf{N}({}^d\boldsymbol{\epsilon})$  so that matter is continuously distributed (de Wit 1970).

The elastic strain  $\boldsymbol{\epsilon}$  is a state function for a crystalline lattice, but the internal  ${}^I\boldsymbol{\epsilon}$  and dislocation  ${}^d\boldsymbol{\epsilon}$  strains are not (de Wit 1970).

[16]: Similarly, the increase in a system's internal energy,  $dE$ , is a state function (exact differential or 1-form) which is given by the sum of two Pfaffians (inexact 1-forms),  $\Delta W$  and  $\Delta q$ , the work done on and the heat absorbed by the system, respectively (Lavenda 1978).

[17]: Also,  $\nabla \times \boldsymbol{\gamma} = -\nabla \times {}^d\boldsymbol{\gamma}$  (Kröner 1959/60).

Now let  $\vec{d}\vec{\omega}^a$  denote the small rotations of the lattice planes associated with the displacement  $\vec{d}x^b$ ; then

$$\vec{d}\vec{\omega}^a = (\partial \vec{\omega}^a / \partial x^b) \vec{d}x^b \equiv \kappa_b^a \vec{d}x^b.$$

Thus,  $\kappa^{ca} \equiv G^{cb} \kappa_b^a$  are components of the *elastic lattice curvature tensor*

$$\begin{aligned} \kappa &\equiv \# \vec{d}\vec{\omega}^a \otimes \mathbf{i}_a \equiv \nabla \vec{\omega}^a \otimes \mathbf{i}_a \equiv \kappa^{ca} \mathbf{i}_c \otimes \mathbf{i}_a; \\ {}^b\kappa &\equiv \vec{d}\vec{\omega}^a \otimes \mathbf{i}_a = \kappa_b^a \vec{d}x^b \otimes \mathbf{i}_a. \end{aligned}$$

Since  $\kappa \equiv \nabla \vec{\omega}^a$ ,  $\nabla \times \kappa = \mathbf{0}$  identically: In a *crystal* the lattice rotation  $\vec{\omega}$  is everywhere single-valued, and therefore (Nabarro 1967)

$$\partial \kappa_b^a / \partial x^c = \partial^2 \vec{\omega}^a / \partial x^c \partial x^b = \partial^2 \vec{\omega}^a / \partial x^b \partial x^c = \partial \kappa_c^a / \partial x^b,$$

which implies that

$$\nabla \times \kappa = \mathbf{0}, \text{ or } \vec{d}{}^b\kappa = \mathbf{0},$$

or

$$\vec{d}^2 \vec{\omega}^a = \mathbf{0}.$$

If, on the other hand, lattice curvature is generated by disclinations, then

$$\Theta \equiv \vec{\nabla} \times {}^b\kappa,$$

$\Theta$  denoting the *disclination density tensor*. The components of  $\Theta$  are (Kröner and Lagoudas 1992).

$$\Theta^{ad} \equiv \epsilon^{abc} \partial_b K_c^d.$$

Huang and Mura (1970) provide a relationship for a circular edge disclination that is analogous to Burgers multivalued displacement function, and with this function  $\kappa$  is not a gradient, its curl is non-zero, and the disclination density  $\Theta$  is non-zero as well.

Since  $\Theta$  is defined as a curl, it will have no "source," *i.e.*

$$\nabla \bullet \Theta = 0,$$

disclination lines do not end in the lattice; they form either closed loops or terminate at the surface of the material.

If there are disclinations in the lattice, the compatibility statement  $\mathbf{N}(\mathcal{E}) = \mathbf{0}$  for the internal strain  $\mathcal{E} \equiv \boldsymbol{\epsilon} + \mathcal{E}$  becomes, instead of  $\vec{\nabla} \times \boldsymbol{\epsilon} \times \vec{\nabla} = -\vec{\nabla} \times \mathcal{E} \times \vec{\nabla} = -{}^{symm}(\nabla \times {}^d\mathbf{p})$ , the following (de Wit 1970):

$$\vec{\nabla} \times \boldsymbol{\epsilon} \times \vec{\nabla} = {}^{symm}(\Theta - \nabla \times {}^d\mathbf{p}).$$

Finally, when there are disclinations in the lattice, then dislocations can end on the disclinations, *i.e.* the dislocation density can diverge (de Wit 1970, Kröner and Lagoudas 1992):

$$\nabla \cdot \rho = \nabla \times \Theta \text{ or, } \partial_d \rho^d_c = \epsilon_{abc} \Theta^{ab}.$$

The *total strain*,  $\tilde{\boldsymbol{\epsilon}}$ , is obtained from measurements on the exterior dimensions of a body before and after deformation; it is therefore a coarser quantity than the strain fields associated with lattice defects (Christian 1965). Unless the material fractures,  $\tilde{\boldsymbol{\epsilon}}$  must be a compatible deformation (Bilby 1960, Christian 1965). The total strain is the sum of elastic and plastic strains,  $\tilde{\boldsymbol{\epsilon}} \equiv \boldsymbol{\epsilon} + \boldsymbol{\epsilon}_p$ , but this is not really a practicable definition (Edelen 1979), *i.e.* it can not be presumed to reflect two distinct measurements. Also, neither plastic or total strains are state functions.

**Plastic strain results when defects traverse the lattice:** *e.g.* dislocation slip. A compatibility argument can be constructed for the flow of a lattice from dislocation motion by utilizing a discussion of hydrodynamics from Schouten (1989). Let the density of the lattice be  $m$  so that  $\int_V m dV = \int_V *m$  is the mass of material in the region  $V$ , where  $*m \equiv m \vec{dx} \wedge \vec{dy} \wedge \vec{dz} \equiv m\epsilon$ . If blocks of material move with some velocity  $v$  then there is a mass flux,  $J$ ,  $J \equiv m v$ ;  $[J] = \text{mass per unit area per unit time}$ . Now  $\star J = J_a \vec{dx}^a$  is the 1-form that corresponds to this flux and,  $\star \star J = J_x \vec{dy} \wedge \vec{dz} + J_y \vec{dz} \wedge \vec{dx} + J_z \vec{dx} \wedge \vec{dy}$  is the "twisted" 2-form (Burke 1985): "tubes" of  $\star \star J$  lie in the direction of mass flow and are sized to unit area.<sup>[18]</sup> The number of particles passing through the boundary  $\partial V$  of  $V$  is  $\int_{\partial V} \star \star J$ , so the

[18]: The flow of electric charge is a "twisted" 2-form: for example, the "tubes" of  $\star \star J$  lie along the current flow, are sized to enclose unit current, and have an orientation given by the direction of the current flow (Burke 1985). I am using the  $\star$  symbol here to denote formation of the "twisted" 2-form from a 1-form. Burke

mass density in  $\mathbf{V}$  changes by  $(\partial/\partial t) \int_{\mathbf{V}} *m = \int_{\mathbf{V}} \partial *m/\partial t$ :  $\int_{\partial\mathbf{V}} \star^b \mathbf{J} = \int_{\mathbf{V}} \partial *m/\partial t$ . The *divergence theorem* (a special case of Stokes' theorem) is  $\int_{\partial\mathbf{V}} \alpha = \int_{\mathbf{V}} \vec{d}\alpha$ , where  $\alpha$  is any 2-form. Thus  $\int_{\partial\mathbf{V}} \star^b \mathbf{J} = \int_{\mathbf{V}} \vec{d}\star^b \mathbf{J} = \int_{\mathbf{V}} \partial *m/\partial t$  and therefore  $\vec{d}\star^b \mathbf{J} = \partial *m/\partial t$ . Since

$$\begin{aligned}\vec{d}\star^b \mathbf{J} &= \vec{d}(J_x \vec{d}y \wedge \vec{d}z + J_y \vec{d}z \wedge \vec{d}x + J_z \vec{d}x \wedge \vec{d}y), \\ &= \sum_a (\partial J_a / \partial x^a) \vec{d}x \wedge \vec{d}y \wedge \vec{d}z, \\ &= (\nabla \bullet \mathbf{J}) \boldsymbol{\epsilon},\end{aligned}$$

the *continuity equation*,  $\nabla \bullet \mathbf{J} = \partial m / \partial t$ , is obtained. If  $\nabla \bullet \mathbf{J} = 0$  the total mass in every  $\boldsymbol{\epsilon}$  is *constant*. The "tubes" are "inpenetrable," meaning that the same mass flows through each section of each "tube" in unit time. The "tubes"  $\star^b \mathbf{J}$  fill space without gaps or overlaps.

Bilby (1960) and his coworkers recognized that *Pfaff's problem* (Schouten and Kulk 1969),  $\vec{d}\chi^\alpha = \lambda^\alpha_a \vec{d}x^a$ , is equivalent to the problem of a dislocation in an elastic continuum. The equation  $\vec{d}\chi^\alpha = \lambda^\alpha_a \vec{d}x^a$  is used in the remaining sections to develop expressions for elastic, dislocation, and total strains in a crystal lattice. Directions characterizing the symmetry of the lattice are natural candidates for a "coordinate system" to represent these deformations and their sources; sources being mostly dislocations, but disclinations are discussed as well. "Singularities," slip planes, and slip directions are easily defined with such coordinates.

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(1985) does not use special notation for these objects, and neither do I in the Appendix where they are discussed further.

### Pfaff's Problem

from Schouten and Kulk (1969)

*"In olden times there was a slave, packing valuable leaves for his king. But he packed the leaves at random and the leaves came out badly damaged and the king was very angry and the head of the slave was cut off. Many other slaves came and went and the story was very sad. But at last there came one more intelligent than his predecessors, who packed the leaves nicely in layers, and they came out in a way that pleased the king. The slave not only saved his own life but he was the first man who faced and solved a Pfaff's problem.*

*Now let us take the leaves very small and very thin, say, infinitesimal 'facets', and let us pack them so closely that there is one facet in every point in the occupied space. Then they may be arranged in such a way that they form a system of  $\infty^1$  surfaces in space. That is the nice packing. But if the packing is at random, though continuous, no such surfaces can be built. That is the packing to be condemned if valuable leaves are concerned. But mathematically it is not less interesting. To handle all kinds of packing we need an exact mathematical formulation and this will be done at once for an  $n$ -dimensional space."*

## 1.6. The Crystallographic Coordinate System

Consider a tensile specimen comprised of a single, stress-free crystal with no defects.

A *crystallographic coordinate system* (Christian 1965)  $X, Y, Z$ , or "manifold," can be embedded in the crystal, Figure 4. The  $X^M$  coordinates are aligned, for example, with the crystallographic directions [100], [010], [001] of a *unit cell*, e.g. the *conventional unit cell*, Figure 5. The crystallographic coordinates  $X^M$  can always be related to those of the  $x^a$  reference frame by a simple relationship like (Christian 1965, Wrede 1972, Schouten 1989)

$$X^M = X^M(x^a) \equiv \lambda_{\alpha}^M x^a, \quad \lambda_{\alpha}^M \equiv \begin{vmatrix} \lambda_x^x & \lambda_x^y & \lambda_x^z \\ \lambda_y^x & \lambda_y^y & \lambda_y^z \\ \lambda_z^x & \lambda_z^y & \lambda_z^z \end{vmatrix},$$

where  $\lambda_{\alpha}^M$  is a *matrix* comprised of nine constants. Therefore, **there is no essential difference between the  $x^a$  reference frame and the  $X^M$  crystallographic coordinates**; these coordinates were written down directly without the intermediate step of solving differential equations.

The *tangent basis vectors* can be taken as the lattice vectors  $\{A_x[100], A_y[010], A_z[001]\} \equiv \{A_M I_M\} \equiv \{A_M\}$ , where, for example,  $I_x \equiv [100]$  is a unit vector in the  $X$ -direction,  $A_x \equiv A_x[100]$  is a *lattice vector* of the conventional unit cell and  $A_x$  is the *lattice parameter*: Each of the vectors  $A_M$  extend from one atom to the next along the crystallographic coordinate  $X^M$ .

Every atom in the crystal is at a point  $\rho$ , or lattice site, with coordinates  $\rho = x^a \mathbf{i}_a$ ; the next atom is located a distance  $d\rho = \mathbf{i}_a dx^a = \mathbf{A}_M dX^M$  away from the first.<sup>[19]</sup> If such a displacement follows a crystallographic coordinate, say  $X$ , then  $d\rho = \mathbf{A}_x dX$ , which implies that the  $\mathbf{A}_M$  are tangent vectors to the respective  $X^M$  coordinate "curves" (Malvern 1969). Thus (since  $d\rho = \mathbf{A}_M dX^M$  or, equivalently,  $\vec{d}\rho = \mathbf{A}_M \vec{d}X^M$ ),

$$\begin{aligned}\mathbf{A}_M &\equiv \partial \rho / \partial X^M = \sum_a (\partial \rho / \partial x^a) (\partial x^a / \partial X^M) = \sum_a \mathbf{i}_a (\partial x^a / \partial X^M), \\ &= (\partial x / \partial X^M) \mathbf{i} + (\partial y / \partial X^M) \mathbf{j} + (\partial z / \partial X^M) \mathbf{k}, \\ &\equiv A_M \mathbf{I}_M \text{ (no sum)},\end{aligned}$$

where  $A_M = [(\partial x / \partial X^M)^2 + (\partial y / \partial X^M)^2 + (\partial z / \partial X^M)^2]^{1/2}$ , and  $\mathbf{i}_a \equiv \partial \rho / \partial x^a \equiv \partial / \partial x^a$ . Equivalently,  $\mathbf{A}_M \equiv \partial / \partial X^M \equiv \vec{\partial}_M$  (Marsden and Hughes 1983), which follows from  $d\rho = \mathbf{A}_M dX^M \rightarrow \mathbf{A}_M = \partial \rho / \partial X^M$  by dropping the argument  $\rho$  from the partial derivative. The units of each  $\mathbf{A}_M$  are  $[\mathbf{A}_M] = [A_M] = \text{distance}$ ; the  $X^M$  and  $\mathbf{I}_M$  are unit-less.<sup>[20]</sup>

For a conventional unit cell each of the vectors  $\mathbf{A}_M$  lies between two planes from the family  $\{(100), (010), (001)\}$ ; e.g. (100) for  $\mathbf{A}_x$ . Thus, pairs of these planes represent the cotangent basis vectors (Schouten 1954, 1989, Nabarro 1967, Misner *et al.* 1973). The *cotangent basis vectors*,  $\mathbf{A}^M$ , are normal to the level surfaces of the  $X^M$ , which are  $X^M \equiv$

[19]: Malvern's term  $d\rho$  is, more rigorously (Misner *et al.* 1973, Flanders 1989):

$d\rho \rightarrow \vec{d}\rho = \vec{d}\rho(\dots, \dots)$ , with  $\vec{d}\rho \equiv \mathbf{i}_a \otimes \vec{d}x^a \equiv \mathbf{A}_M \otimes \vec{d}X^M$ .

[20]: The notion that coordinates serve to measure distance has therefore been given up (Misner *et al.* 1973).

constants, and the normal vector to such a surface is just (Malvern 1969)

$$\mathbf{A}^M \equiv \nabla X^M \equiv \vec{d}X^M = \sum_a (\partial X^M / \partial x^a) \mathbf{i}^a \equiv \sum_a (\partial X^M / \partial x^a) \vec{d}x^a \equiv \lambda^M_a \vec{d}x^a,$$

since for the last step,  $X^M \equiv \lambda^M_a x^a$ . Note that the cotangent basis vectors  $\vec{d}X^M \equiv \mathbf{A}^M$  have also been given a matrix representation by the identification  $\vec{d}X^M = \lambda^M_a \vec{d}x^a$ . They are not unit normal vectors to their respective planes:  $\mathbf{A}^M \equiv A^M \mathbf{I}^M$ , where, for example,  $\mathbf{I}^x = (100)$ , and in general  $\mathbf{I}^M = \{100\}$  are the unit vectors. The definition  $\mathbf{A}^M \equiv \vec{d}X^M \equiv (\partial X^M / \partial x^a) \vec{d}x^a$  indicates that  $[\mathbf{A}^M] = 1/\text{distance}$ , since the  $\vec{d}x^a \equiv \mathbf{i}^a$  are unitless. Tangent and cotangent basis vectors are "duals," therefore  $\mathbf{A}_M \bullet \mathbf{A}^N = A_M A^N \mathbf{I}_M \bullet \mathbf{I}^N = A_M A^N \delta_{M^N} = A_M A^M \equiv 1$ . Conventional unit cells are orthogonal, and therefore  $A_M = 1/A^M$ ;  $\mathbf{A}^x = (100)/A_x$ .

The *metric tensor*,  $\mathbf{G}$ , for the crystallographic coordinates  $X^M$  of a conventional unit cell is  $\mathbf{G} \equiv \mathbf{1} \equiv \delta_{MN} \mathbf{I}^M \otimes \mathbf{I}^N$ , or equivalently

$$\mathbf{G} \equiv A_x \vec{d}X \otimes A_x \vec{d}X + A_y \vec{d}Y \otimes A_y \vec{d}Y + A_z \vec{d}Z \otimes A_z \vec{d}Z \equiv G_{MN} \vec{d}X^M \otimes \vec{d}X^N.$$

The covariant components of  $\mathbf{G}$  are  $G_{MN} \equiv \mathbf{G}(\vec{d}_M, \vec{d}_N) \equiv \mathbf{A}_M \bullet \mathbf{A}_N = A_M A_N \delta_{M^N} = A_x^2, A_y^2, A_z^2 = G_{xx}, G_{yy}, G_{zz}$ , since the  $X^M$  coordinates are orthogonal. These components are a matrix representation for  $\mathbf{G}$ ,

$$G_{MN} \equiv \begin{vmatrix} G_{xx} & 0 & 0 \\ 0 & G_{yy} & 0 \\ 0 & 0 & G_{zz} \end{vmatrix}.$$

The determinant of this matrix, say  $|G_{MN}|$ , is denoted  $G$ ,  $G \equiv |G_{MN}|$ , and it has the trivial value  $G = G_{xx}G_{yy}G_{zz} = (A_x A_y A_z)^2$  for orthogonal coordinates, also being equivalent to  $(\mathbf{A}_x \bullet \mathbf{A}_y \times \mathbf{A}_z)^2$ . Contravariant components of  $\mathbf{G}$  are  $G^{MN} \equiv \mathbf{A}^M \bullet \mathbf{A}^N$  (Gairola 1979). The relationships

$$G^{MN} G_{NP} = \delta^M_P$$

hold even if the coordinates are not orthogonal (Schouten (1989)). The matrix representation of  $G^{MN}$  is

$$G^{MN} \equiv \begin{vmatrix} G^{xx} & 0 & 0 \\ 0 & G^{yy} & 0 \\ 0 & 0 & G^{zz} \end{vmatrix}$$

for orthogonal coordinates, and the determinant of this matrix is  $|G^{MN}| = G^{-1}$ :  $|G_{MN}| |G^{MN}| = 1$  always holds, so the matrices  $G^{MN}$  and  $G_{MN}$  are always inverses of one another,  $\|G^{MN}\| \equiv \|G_{MN}\|^{-1}$  (Misner *et al.* 1973).

For the Levi-Cevita tensor,  $*1 \equiv \epsilon \equiv \mathbf{I}^x \wedge \mathbf{I}^y \wedge \mathbf{I}^z$ :

$$\begin{aligned} \epsilon &\equiv \epsilon_{LMN} \vec{d}X^L \wedge \vec{d}X^M \wedge \vec{d}X^N \equiv A_x \vec{d}X \wedge A_y \vec{d}Y \wedge A_z \vec{d}Z \equiv G^{1/2} \vec{d}X \wedge \vec{d}Y \wedge \vec{d}Z, \\ &\equiv G^{1/2} e_{LMN} \vec{d}X^L \wedge \vec{d}X^M \wedge \vec{d}X^N; \end{aligned}$$

with the covariant components of  $\epsilon$ ,  $\epsilon_{LMN}$ , being  $\epsilon_{LMN} = G^{1/2} e_{LMN}$ ,  $e_{LMN}$  again denoting the covariant components of the permutation tensor (Malvern 1969). When the basis vectors are

installed,  $\epsilon(\vec{\partial}_x, \vec{\partial}_y, \vec{\partial}_z) = G^{1/2} \vec{d}X(\vec{\partial}_x) \wedge \vec{d}Y(\vec{\partial}_y) \wedge \vec{d}Z(\vec{\partial}_z) \equiv \mathbf{A}_x \bullet \mathbf{A}_y \times \mathbf{A}_z = G^{1/2}$ . Since the conventional unit cell is orthogonal,  $G^{1/2} = A_x A_y A_z$ ;  $[G^{1/2}] = volume$ .

When the  $\mathbf{A}_M$  are primitive lattice vectors the  $\mathbf{A}^M$  define the *reciprocal lattice*. The *primitive unit cell* is a unit cell containing only one corpuscle. The usual definition of the reciprocal lattice vectors  $\mathbf{A}^M$  in terms of the primitive lattice vectors  $\mathbf{A}_M$  is (Christian 1965):

$$\mathbf{A}^x = (\mathbf{A}_y \times \mathbf{A}_z)/[\mathbf{A}_x \bullet \mathbf{A}_y \times \mathbf{A}_z],$$

$$\mathbf{A}^y = (\mathbf{A}_z \times \mathbf{A}_x)/[\mathbf{A}_x \bullet \mathbf{A}_y \times \mathbf{A}_z],$$

$$\mathbf{A}^z = (\mathbf{A}_x \times \mathbf{A}_y)/[\mathbf{A}_x \bullet \mathbf{A}_y \times \mathbf{A}_z].$$

This also works for any *allowable* coordinates,<sup>[21]</sup> orthogonal or non-orthogonal. These relationships can be expressed as

$$\mathbf{A}_L \times \mathbf{A}_M = \epsilon_{LMN} \mathbf{A}^N, \mathbf{A}^L \times \mathbf{A}^M = \epsilon^{LMN} \mathbf{A}_N \text{ and, } \mathbf{A}^L = \frac{1}{2} \epsilon^{LMN} \mathbf{A}_M \times \mathbf{A}_N,$$

where

$$\epsilon^{LMN} \equiv G^{-1/2} e^{LMN} \equiv \Omega_0^{-1} e^{LMN}$$

are the contravariant components of  $\epsilon$ ,  $e^{LMN}$  is the contravariant permutation symbol (Malvern 1969, Gairola 1979);  $\Omega_0 \equiv G^{1/2}$  holds for primitive unit cells,  $\Omega_0$  denoting the *atomic volume*.

[21]: So long as the unit cell is not "flattened," its coordinates are allowable, *i.e.* the basis vectors  $\mathbf{A}_M$  are linearly independent (Misner *et al.* 1973), *i.e.*  $\mathbf{A}_x \bullet \mathbf{A}_y \times \mathbf{A}_z \neq 0$ .

The vectors  $\mathbf{A}_M$  for the body-centered cubic (BCC), face-centered cubic (FCC), and hexagonal close-packed (HCP) primitive unit cells are non-orthogonal.<sup>[22]</sup> Unit vectors  $\mathbf{i}_M$  for primitive unit cells do not correspond to crystallographic directions from the family  $\langle 100 \rangle$ , and similarly the  $\mathbf{i}^M$  do not correspond to planes from the family  $\{100\}$ . The metric tensor of the non-orthogonal coordinates  $X^M$  based on a primitive unit cell is

$$\mathbf{G} \equiv G_{MN} \vec{\mathbf{d}}X^M \otimes \vec{\mathbf{d}}X^N,$$

where

$$G_{NM} = G_{MN} \equiv \mathbf{G}(\vec{\mathbf{d}}_M, \vec{\mathbf{d}}_N) \equiv \mathbf{A}_M \bullet \mathbf{A}_N = A_M A_N \cos \theta,$$

$\theta$  denoting the angle between the two vectors, or equivalently (Malvern 1969)

$$\begin{aligned} G_{MN} &\equiv [\sum_a \mathbf{i}_a (\partial x^a / \partial X^M)] \bullet [\sum_b \mathbf{i}_b (\partial x^b / \partial X^N)], \\ &= (\partial x^a / \partial X^M)(\partial x^b / \partial X^N) \delta_{ab}, \\ &= (\partial x / \partial X^M)(\partial x / \partial X^N) + (\partial y / \partial X^M)(\partial y / \partial X^N) + (\partial z / \partial X^M)(\partial z / \partial X^N). \end{aligned}$$

The metric tensor  $\mathbf{G}$  has six different, non-zero components for non-orthogonal coordinates:  $G_{xx}$ ,  $G_{yy}$ ,  $G_{zz}$ ,  $G_{xy}$ ,  $G_{yz}$ , and  $G_{xz}$ . So the matrix representation of the covariant components of  $\mathbf{G}$ ,  $G_{MN}$ , is

[22]: See in particular Malvern (1969) and Wrede (1972) for introductory accounts of non-orthogonal coordinates, and Schouten (1954, 1989), Misner and Wheeler (1957), Eringen (1971), and Misner *et al.* (1973) for more advanced treatments.

$$G_{MN} = \begin{vmatrix} G_{XX} & G_{YX} & G_{ZX} \\ G_{XY} & G_{YY} & G_{ZY} \\ G_{XZ} & G_{YZ} & G_{ZZ} \end{vmatrix}.$$

The determinant of this matrix is again denoted by  $G$ , and it has the value

$$G \equiv e^{ORS} G_{XQ} G_{YR} G_{ZS} = (\mathbf{A}_x \bullet \mathbf{A}_y \times \mathbf{A}_z)^2;$$

but unlike the orthogonal case,  $G \neq (A_x A_y A_z)^2$ . Contravariant components of  $\mathbf{G}$  are again  $G^{MN} \equiv \mathbf{A}^M \bullet \mathbf{A}^N$ , and the determinant of this matrix is  $|G^{MN}| = G^{-1}$ ;  $G^{MN} G_{NP} = \delta^M{}_P$ ,  $|G_{MN}| |G^{MN}| = 1$ , so  $\|G^{MN}\| \equiv \|G_{MN}\|^{-1}$  (Misner *et al.* 1973). Similarly,

$$\epsilon \equiv A_x \vec{\mathbf{d}} X \wedge A_y \vec{\mathbf{d}} Y \wedge A_z \vec{\mathbf{d}} Z = G^{1/2} \vec{\mathbf{d}} X \wedge \vec{\mathbf{d}} Y \wedge \vec{\mathbf{d}} Z,$$

and  $\epsilon(\vec{\sigma}_x, \vec{\sigma}_y, \vec{\sigma}_z) = G^{1/2}$ . Thus, covariant components of  $\epsilon$ ,  $\epsilon_{LMN}$ , are always (Malvern 1969)

$$\epsilon_{LMN} = G^{1/2} e_{LMN}.$$

For any coordinates in which the  $\mathbf{A}_M \equiv \vec{\sigma}_M$  are primitive lattice vectors,

$$\epsilon(\vec{\sigma}_x, \vec{\sigma}_y, \vec{\sigma}_z) = G^{1/2} \equiv \Omega_0.$$

Thus, the covariant components of  $\epsilon$  are in this case  $\epsilon_{LMN} = G^{1/2} e_{LMN} \equiv \Omega_0 e_{LMN}$ .

The inner product of  $\mathbf{A}_M$  and  $\mathbf{A}^N$  is always (Malvern 1969)

$$\begin{aligned}\mathbf{A}_M \cdot \mathbf{A}^N &= [\sum_a \mathbf{i}_a (\partial x^a / \partial X^M)] [\sum_b (\partial X^N / \partial x^b) \mathbf{i}^b] = \sum_{a,b} [(\partial x^a / \partial X^M)(\partial X^N / \partial x^b)] \mathbf{i}_a \cdot \mathbf{i}^b, \\ &= \sum_{a,b} [(\partial x^a / \partial X^M)(\partial X^N / \partial x^b)] \delta_{a,b} = \delta_M^N;\end{aligned}$$

or equivalently (Misner *et al.* 1973, Marsden and Hughes 1983)

$$\mathbf{A}_M \cdot \mathbf{A}^N \equiv \langle \vec{d}X^N, \partial / \partial X^M \rangle \equiv \vec{d}_{X^M}(\vec{d}X^N) = \partial X^N / \partial X^M = \delta_M^N.$$

Thus the tangent  $\mathbf{A}_M$  and cotangent  $\mathbf{A}^M$  basis vectors are always *dual bases*. If  $\theta$  is the angle between them, then  $\mathbf{A}_M \cdot \mathbf{A}^N = A_M A^M \cos \theta = 1$ . Conventional unit cells for the simple cubic, BCC, and FCC crystal structures are all *orthogonal*, so  $\cos \theta = 1$ , and  $A^M = A_M^{-1}$ . Therefore, only for conventional unit cells do the planes  $X^M = \text{constant}$  have a spacing of  $A^M = A_M^{-1}$ .

The tangent basis vectors  $\mathbf{A}_M$  can also be given a matrix representation: Since  $X^M = \lambda_M^a x^b$ , let  $\lambda_M^a \equiv [\lambda_M^a]^{-1}$ , i.e.  $\lambda_M^a X^M = \lambda_M^a \lambda_M^b x^b \equiv \delta_a^b x^b = x^a$ , so that  $\lambda_M^a = \partial x^a / \partial X^M$ . Thus,

$$x^a = \lambda_M^a X^M, \text{ and } \lambda_M^a \equiv \left[ \begin{array}{ccc} \lambda_x^x & \lambda_y^x & \lambda_z^x \\ \lambda_x^y & \lambda_y^y & \lambda_z^y \\ \lambda_x^z & \lambda_y^z & \lambda_z^z \end{array} \right];$$

therefore

$$\mathbf{A}_M \equiv (\partial x^a / \partial X^M) \mathbf{i}_a \equiv \lambda_M^a \mathbf{i}_a.$$

In addition to  $\lambda_M^a \lambda^M_b = \delta^a_b$ , the relationships  $\lambda^M_a \lambda_N^a = \delta^M_N$  also hold. The matrices  $\lambda^M_a$  and  $\lambda_M^a$  are also related by (Schouten 1989)

$$\lambda_M^a \equiv |\text{minor}(\lambda^M_a)| / |\lambda^M_a|.$$

Here, the minor of  $\lambda^M_a$ ,  $\text{minor}(\lambda^M_a)$ , is the  $2 \times 2$  matrix obtained from  $\lambda^M_a$  by striking out the  $M$ -th column and  $a$ -th row and multiplying by  $(-1)^{M+a}$ , and the vertical bars mean take the determinant of this matrix. The determinant of  $\lambda^M_a$  is

$$|\lambda^M_a| \equiv e_{MNP} \lambda^M_1 \lambda^N_2 \lambda^P_3 \equiv \mathbf{A}^x \bullet \mathbf{A}^y \times \mathbf{A}^z = G^{-1/2},$$

which is  $\Omega_0^{-1}$  when the  $\mathbf{A}^M$  are primitive cotangent basis vectors; the determinant of  $\lambda_M^a$  is

$$|\lambda_M^a| \equiv e^{MNP} \lambda_M^1 \lambda_N^2 \lambda_P^3 \equiv \mathbf{A}_x \bullet \mathbf{A}_y \times \mathbf{A}_z = G^{1/2}.$$

The *Wigner-Seitz primitive cell*, Figure 6, contains the region of space around a lattice site that is closer to the site than to any other in the lattice. The Wigner-Seitz primitive cells surrounding each atom in a BCC lattice are tetrakaidecahedrons (Ashcroft and Mermin 1976). Wigner-Seitz primitive cells are hexagons for a lattice with *sixfold* symmetry.

Now consider a polycrystalline tensile specimen with a small enough grain size to undergo creep or superplastic deformation. A simple model of a polycrystalline material is a uniform array of tetrakaidecahedrons. The corpuscles are now grains, but they are modelled as these three dimensional cells; constituents of the grains (*e.g.* atoms and dislocations) are ignored in this level of description. The "dual" lattice corresponding to this cellular array (stack of tetrakaidecahedrons) is BCC (Morral and Ashby 1974): each cell "contains" one point from the BCC lattice for which it is a Wigner-Seitz primitive cell. Attention can therefore be focussed on the cells, or the points in a BCC lattice with, for example, conventional unit cell vectors  $\mathbf{A}_M$ ;  $A_x = A_y = A_z \equiv A$ . These  $\mathbf{A}_M$  are orthogonal, and their dimensions are  $\mu\text{m}$ . The cotangent vectors  $\mathbf{A}^M$  represent (100),(010),(001) planes for  $\mathbf{A}^x, \mathbf{A}^y, \mathbf{A}^z$ ;  $A^x = A^y = A^z = 1/A$ , *i.e.* the separation between planes of type {100} is  $A$ . The volume of the conventional unit cell is  $G^{1/2} \equiv \epsilon(\vec{\mathcal{D}}_x, \vec{\mathcal{D}}_y, \vec{\mathcal{D}}_z) \equiv \mathbf{A}_x \cdot \mathbf{A}_y \times \mathbf{A}_z = A^3 \mu\text{m}^3$ , which is twice the volume of a tetrakaidecahedron.

The *number of cells per unit volume* is  $N_v = 2/A^3$ ; *cell boundary area per unit volume* is  $A_v = 3.35/A$ ; *cell edge length per unit volume* is  $L_v = 8.5/A^2$ ; and the *number of cell corners per unit volume* is  $C_v = 12/A^3$  (Christian 1965).

Corners are also referred to as *vertices*.

**Summary of Section 1:** Some mathematics is summarized in the next box, mostly after Abraham *et al.* (1988). Figure 7 provides illustrations of Pfaff's problem (curl, rotation, and the Frobenius theorem), divergence, the Bianchi identity, and the metric tensor.

### Summary Definitions

<b>Vector</b>	$\mathbf{v} = v^M \mathbf{A}_M \equiv v^M \vec{d}_M; \# \alpha \equiv \alpha^M \mathbf{A}_M$ , where $\alpha^M \equiv G^{MN} \alpha_N$ .
<b>1-form</b>	$\alpha = \alpha_M \mathbf{A}^M \equiv \alpha_M \vec{d} X^M$ and ${}^b \mathbf{v} \equiv v_M \mathbf{A}^M$ are covariant vectors;
	$v_M = G_{MN} v^N, v^M = G^{MN} v_N$ .
<b>2-form</b>	$\mathbf{B} = \beta_{[MN]} \vec{d} X^M \wedge \vec{d} X^N = \frac{1}{2} \beta_{MN} \vec{d} X^M \wedge \vec{d} X^N; \beta_{MN} = -\beta_{NM}$ .
<b>3-form</b>	$\gamma = \gamma_{[MNP]} \vec{d} X^M \wedge \vec{d} X^N \wedge \vec{d} X^P = \frac{1}{3} \gamma_{MNP} \vec{d} X^M \wedge \vec{d} X^N \wedge \vec{d} X^P$ .
<b>Levi-Cevita</b>	$\epsilon \equiv G^{1/2} \epsilon_{MNP} \vec{d} X^M \wedge \vec{d} X^N \wedge \vec{d} X^P; G =  G_{MN} $ ;
<b>Tensor</b>	$e_{MNP} = 1 (-1)$ for even (odd) permutation of MNP, $e_{MNP} = 0$ if any two indices are the same.
<b>* Operator</b>	$*f \equiv f(\vec{d} X \wedge \vec{d} Y \wedge \vec{d} Z); \alpha = \alpha_M \vec{d} X^M \Rightarrow * \alpha = \alpha^M \epsilon_{MNP} \vec{d} X^N \wedge \vec{d} X^P;$ $\mathbf{B} = \frac{1}{2} \beta_{MN} \vec{d} X^M \wedge \vec{d} X^N \Rightarrow * \mathbf{B} = \frac{1}{2} \beta^{MN} \epsilon_{MNP} \vec{d} X^P$ .
<b>Cross Product</b>	$\mathbf{u} \times \mathbf{v} \equiv \#[*({}^b \mathbf{u} \wedge {}^b \mathbf{v})]$ .
<b>Dot Product</b>	$(\mathbf{u} \cdot \mathbf{v}) \vec{d} x \wedge \vec{d} y \wedge \vec{d} z \equiv {}^b \mathbf{u} \wedge *({}^b \mathbf{v})$ .
<b>Gradient</b>	$\#(\vec{d} f) \equiv \nabla f \equiv G^{MN} (\partial f / \partial X^N) \mathbf{A}_M; {}^b \nabla f = \vec{d} f$ .
<b>Rotation</b>	$\text{rot } \mathbf{v} \equiv \vec{d} {}^b \mathbf{v} \equiv (\partial v_a / \partial x^b) \vec{d} x^b \wedge \vec{d} x^a$ $= \frac{1}{2} (\partial v_a / \partial x^b - \partial v_b / \partial x^a) \vec{d} x^b \wedge \vec{d} x^a$ , $\equiv (\partial v_z / \partial y - \partial v_y / \partial z) \vec{d} y \wedge \vec{d} z$ $+ (\partial v_x / \partial z - \partial v_z / \partial x) \vec{d} z \wedge \vec{d} x$ $+ (\partial v_y / \partial x - \partial v_x / \partial y) \vec{d} x \wedge \vec{d} y$ .
<b>Curl</b>	$\text{curl } \mathbf{v} = \nabla \times {}^b \mathbf{v} \equiv \#[*(\vec{d} {}^b \mathbf{v})] = \#[*(\text{rot } \mathbf{v})]$ .
<b>Divergence</b>	$\text{div } \mathbf{v} = \nabla \cdot {}^b \mathbf{v} \equiv * \vec{d} [*({}^b \mathbf{v})]$ .

## §2. Stretching Unit Cells—Elasticity

*"Dislocations destroy translational long range order. Therefore a crystallographic system of coordinates may be introduced only locally, since certain crystallographic planes may vanish inside the crystal terminating on dislocations."* From Dzyaloshinskii and Volovick (1980).

The lattice can be deformed elastically by either internal or external loads. External loads are applied by the experimenter while internal loads are applied by defects in the lattice; these defects are dislocations (Frank 1951) and disclinations (Frank 1958). Elastic deformations are so small that nowhere in the lattice are there any sites that have been rearranged: in other words, no corpuscles have been moved so far as to fall into another position of the same symmetry. See Krishnan and Rajagopal (1961) for a full accounting of the atomistic and continuum theories of crystal elasticity.

Coordinates  $X^M$  with tangent  $\mathbf{A}_M \equiv \partial/\partial X^M$  and cotangent  $\mathbf{A}^M \equiv \vec{d}X^M$  basis vectors are for an ideal lattice representing a tensile specimen prior to any deformation. When a small load is applied to the specimen a *displacement field*  $\mathbf{u}(x^a) = \mathbf{u}(X^M)$  develops throughout it, Figure 8. The initial coordinates  $X^M$  are *dragged* over  $\mathbf{u}$  to new coordinates  $x^m$ ; but the coordinates are otherwise unaffected by this process; they have the same values as before the deformation,  $\{x,y,z\} = \{X,Y,Z\}$  (Eshelby 1956, Schouten 1989, Marcinkowski 1979, Kröner 1992):

$$x^m = \delta^m_M X^M, \text{ and } X^M = \delta^M_m x^m.$$

Basis vectors  $\mathbf{A}_M$  for the original lattice are orthogonal only for BCC and FCC conventional unit cells. In general the "new" tangent,  $\mathbf{a}_m \equiv \partial/\partial x^m$ , and cotangent,  $\mathbf{a}^m \equiv \vec{d}x^m$ , basis vectors for the deformed crystal structure will not be orthogonal.<sup>[23]</sup> Let  $\mathbf{i}_m$  and  $\mathbf{i}^m$  denote unit vectors for the  $x^m$  coordinates of the deformed crystal structure. This coordinate system has a metric tensor  $\mathbf{g} \equiv \delta_{mn} \mathbf{i}^m \otimes \mathbf{i}^n$ , or equivalently  $\mathbf{g} \equiv g_{mn} \vec{d}x^m \otimes \vec{d}x^n$ . Covariant components of  $\mathbf{g}$  are  $g_{nm} = g_{mn} \equiv g(\vec{d}_m, \vec{d}_n) \equiv \mathbf{a}_m \cdot \mathbf{a}_n = a_m a_n \cos \theta$ ,  $\theta$  denoting the angle between  $\mathbf{a}_m$  and  $\mathbf{a}_n$ , where  $\mathbf{a}_m \equiv \partial \rho / \partial x^m \equiv a_m \mathbf{i}_m \equiv \partial / \partial x^m \equiv \vec{d}_m$ , and  $\mathbf{a}^m \equiv {}^b \nabla x^m = \sum_a (\partial x^m / \partial x^a) \mathbf{i}^a \equiv (\partial x^m / \partial x^a) \mathbf{i}^a \equiv \vec{d}x^m$ . The determinant of the matrix  $g_{mn}$ ,  $|g_{mn}|$ , is  $|g_{mn}| = (\mathbf{a}_x \cdot \mathbf{a}_y \times \mathbf{a}_z)^2 \equiv g$ ;  $g \neq (a_x a_y a_z)^2$  generally because the  $x^m$  are probably not orthogonal. Contravariant components of  $\mathbf{g}$  are  $g^{mn} \equiv \mathbf{a}^m \cdot \mathbf{a}^n$ ;  $|g^{mn}| = g^{-1}$ ,  $g^{mn} g_{np} = \delta_p^m$ ,  $|g_{mn}| |g^{mn}| = 1$ , and  $\|g^{mn}\| \equiv \|g_{mn}\|^{-1}$  (Misner *et al.* 1973). The Levi-Cevita tensor is again  $*1 = \epsilon$ , where

[23]: Lower-case letters  $x, y, z$  are for the coordinates  $x^a$  of the reference frame, which has unit vectors  $\mathbf{i}_a \equiv \partial/\partial x^a$  and  $\mathbf{i}^a \equiv \vec{d}x^a$ , sub-and superscripts being denoted with lower-case letters from the beginning of the alphabet. Upper-case letters are for the undeformed crystallographic coordinates  $X^M$ , which have unit vectors  $\mathbf{I}_M$  and  $\mathbf{I}^M$ , sub-and superscripts being denoted with upper-case letters from the middle of the alphabet. Lower-case letters are also for the deformed crystallographic coordinates  $x^m$ , which have unit vectors  $\mathbf{i}_m$  and  $\mathbf{i}^m$ , sub-and superscripts being denoted with lower-case letters from the middle of the alphabet.

$$\begin{aligned}\epsilon &\equiv \epsilon_{lmn} \vec{dx}^l \wedge \vec{dx}^m \wedge \vec{dx}^n \equiv a_x \vec{dx} \wedge a_y \vec{dy} \wedge a_z \vec{dz} \equiv g^{1/2} \vec{dx} \wedge \vec{dy} \wedge \vec{dz}, \\ &\equiv g^{1/2} e_{lmn} \vec{dx}^l \wedge \vec{dx}^m \wedge \vec{dx}^n;\end{aligned}$$

the covariant components of  $\epsilon$ ,  $\epsilon_{lmn}$ , are  $\epsilon_{lmn} = g^{1/2} e_{lmn}$ . When the basis vectors are installed,  $\epsilon(\vec{\partial}_x, \vec{\partial}_y, \vec{\partial}_z) \equiv \mathbf{a}_x \bullet \mathbf{a}_y \times \mathbf{a}_z = g^{1/2}$ . If the  $\mathbf{a}_m$  are for a primitive unit cell, then  $\epsilon(\vec{\partial}_x, \vec{\partial}_y, \vec{\partial}_z) \equiv \mathbf{a}_x \bullet \mathbf{a}_y \times \mathbf{a}_z = g^{1/2} \equiv \Omega$  is the atomic volume in the elastically deformed condition. The atomic volume can be increased by a *tensile* elastic deformation,  $\Omega > \Omega_0$ , and decreased by a *compressive* elastic deformation,  $\Omega < \Omega_0$ .

The *non-linear elastic strain tensor*,  $\boldsymbol{\epsilon}$ , is given by one-half the difference between the new metric and the old metric for a given unit cell:  $\boldsymbol{\epsilon} \equiv \frac{1}{2}(g - G)$ . In order to use this equation one metric must be expressed in terms of the other's coordinates. "New" cotangent basis vectors  $\vec{dx}^m \equiv \mathbf{a}^m$  for the deformed coordinates ( $x^m$ ) can be related to the "old" ones  $\vec{d}X^M \equiv \mathbf{A}^M$  for the undeformed coordinates ( $X^M$ ) by (Kröner 1992)

$$\vec{dx}^m = \lambda^m_M \vec{d}X^M \text{ and, } \vec{d}X^M = \lambda_m^M \vec{dx}^m.$$

Similarly for the tangent basis vectors (Schouten 1989):

$$\partial/\partial x^m \equiv \vec{\partial}_m \equiv \mathbf{a}_m = \lambda_m^M \mathbf{A}_M, \text{ and } \partial/\partial X^M \equiv \vec{\partial}_M \equiv \mathbf{A}_M = \lambda^m_M \mathbf{a}_m.$$

The  $\lambda^m_M$  matrix can be used to express the metric  $g$  of the  $x^m$  coordinates in terms of the original  $X^M$  coordinates:

$$\mathbf{g} = g_{mn} \vec{\mathbf{d}}x^m \otimes \vec{\mathbf{d}}x^n = g_{mn} (\lambda^m{}_M \vec{\mathbf{d}}X^M) \otimes (\lambda^n{}_N \vec{\mathbf{d}}X^N) = g_{mn} \lambda^m{}_M \lambda^n{}_N \vec{\mathbf{d}}X^M \otimes \vec{\mathbf{d}}X^N.$$

$$\equiv g_{MN} \vec{\mathbf{d}}X^M \otimes \vec{\mathbf{d}}X^N.$$

Then the strain tensor can be reexpressed as

$$\boldsymbol{\epsilon} \equiv \frac{1}{2}(\mathbf{g} - \mathbf{G}) = \frac{1}{2}(g_{MN} - G_{MN}) \vec{\mathbf{d}}X^M \otimes \vec{\mathbf{d}}X^N.$$

In order for the strain to be integrable so that the resulting displacements can be determined from it, compatibility conditions must be met (Malvern 1969). The compatibility conditions for the strain are expressed with the incompatibility tensor,

$$\mathbf{N} \equiv N^{ab} \mathbf{i}_a \otimes \mathbf{i}_b \equiv -\vec{\nabla} \times \boldsymbol{\epsilon} \times \hat{\nabla}.$$

This tensor has components

$$N^{ab} = -\boldsymbol{\epsilon}^{acc} \boldsymbol{\epsilon}^{bdf} \partial_c \partial_d \boldsymbol{\epsilon}_{ef},$$

in the reference frame  $\{x^a\}$ , where  $\partial_a \equiv \partial/\partial x^a$  (Kröner 1992), and

$$N^{ij} = -\boldsymbol{\epsilon}^{ikm} \boldsymbol{\epsilon}^{jln} \boldsymbol{\epsilon}_{mn;lk},$$

in the deformed coordinates  $\{x^m\}$ , where  $\nabla \times \mathbf{v} \equiv \boldsymbol{\epsilon}^{ijk} v_{k;j} \mathbf{a}_i$  is the *curl* of a covariant vector  ${}^b \mathbf{v} = v_k \mathbf{a}^k$ ,  $v_{k;l}$  denotes components for the *covariant derivative*  $\nabla$  (Malvern 1969), *e.g.*

$$\nabla_{a_i} {}^b \mathbf{v} \equiv \nabla {}^b \mathbf{v}(\dots, \mathbf{a}_i) \equiv [\partial v_k / \partial x^l - v_q \Gamma^q{}_{kl}] \mathbf{a}^k$$

(Misner *et al.* 1973), and therefore

$$\nabla_{\mathbf{a}_l} \boldsymbol{\varepsilon} = [\partial \varepsilon_{mn}/\partial x^l - \Gamma_{ml}^q \varepsilon_{qn} - \Gamma_{nl}^q \varepsilon_{mq}] \mathbf{a}^m \otimes \mathbf{a}^n.$$

The quantities  $\Gamma_{np}^m$  are *connection coefficients*; they are the components of the covariant derivative operator  $\nabla$  (Misner *et al.* 1973) and tell how the basis vectors  $\mathbf{a}_m$  (or  $\mathbf{a}^m$ ) "bend" through space  $\{x^a\}$  (Misner and Wheeler 1957):

$$\Gamma_{np}^m \equiv \langle \vec{d}x^m, \nabla_{\mathbf{a}_p} \mathbf{a}_n \rangle = -\langle \nabla_{\mathbf{a}_p} \mathbf{a}^m, \mathbf{a}_n \rangle \Rightarrow \nabla_{\mathbf{a}_p} \mathbf{a}_n = \Gamma_{np}^m \mathbf{a}_m \text{ and } \nabla_{\mathbf{a}_p} \mathbf{a}^m = -\Gamma_{np}^m \mathbf{a}^n.$$

The covariant derivative is illustrated by Figure 9.<sup>[24]</sup> The tensor  $\mathbf{N}$  is

$$\mathbf{N} = -\epsilon^{ikm} \epsilon^{jln} \varepsilon_{mn;lk} \mathbf{a}_i \otimes \mathbf{a}_j = -\vec{V} \times \boldsymbol{\varepsilon} \times \hat{\vec{V}};$$

its components are  $N^{ij} = -g^{-1}[\varepsilon_{mn;lk} - \varepsilon_{kn;lm} - \varepsilon_{ml;nk} + \varepsilon_{kl;nm}]^{ij}$ . If  $\mathbf{N} = \mathbf{0}$  then the linear part of  $\boldsymbol{\varepsilon}$  is *compatible*: Cut the material up into cubes and then apply a strain to each one. The cubes probably will not fit back together again without leaving gaps unless further

[24]: For any function  $f$  the covariant and exterior derivatives are the same (Misner *et al.* 1973):

$$\vec{d}f = \nabla f = (\partial f / \partial x^m) \vec{d}x^m = \partial_m f \mathbf{a}^m.$$

**The covariant derivative is a generalization of the gradient operator; it differentiates basis vectors** (e.g.  $\mathbf{a}_m$  and  $\mathbf{a}^m$ ). See the appendix for full details and the upcoming box for a brief introduction.

strains are applied to them; but if they all do fit together again, then  $\mathbf{N} = \mathbf{0}$  and the strain is compatible (Malvern 1969). Compatibility is illustrated by Figure 10. "Incompatibility arises when non-fitting material elements are forced by elastic deformation to form a compact body" (Kröner 1992). An incompatible situation is described by  $\mathbf{N} \neq \mathbf{0}$ .

### "Coordinate Transformations"

The relationships

$$\vec{dx}^m = \lambda^m_M \vec{d}X^M, \text{ and } \vec{d}X^M = \lambda_m^M \vec{d}x^m,$$

and

$$\mathbf{a}_m = \lambda_m^M \mathbf{A}_M, \text{ and } \mathbf{A}_M = \lambda^m_M \mathbf{a}_m,$$

(or equivalently

$$\partial/\partial x^m = \lambda_m^M \partial/\partial X^M, \text{ and } \partial/\partial X^M = \lambda^m_M \partial/\partial x^m)$$

are examples of "coordinate transformations" (Misner *et al.* 1973). The  $\lambda^m_M$  are functions of the undeformed  $X^M$  coordinates (Marsden and Hughes 1983). Contravariant components "transform" like

$$v^m = \lambda^m_M v^M, \text{ and } v^M = \lambda_m^M v^m,$$

since  $\lambda_m^M \lambda^m_N = \delta_m^N$  (Schouten 1989). The  $\lambda_m^M$  are functions of the deformed  $x^m$  coordinates (Marsden and Hughes 1983). Covariant quantities "transform" like

$$\omega_m = \lambda_m^M \omega_M, \text{ and } \omega_M = \lambda^m_M \omega_m,$$

since  $\lambda^m_M \lambda_m^N = \delta_M^N$  (Schouten 1989).

### Coefficients of an Affine Connection

The connection coefficients are components of the covariant derivative, or *connection*,  $\nabla$  (Misner *et al.* 1973):

$$\Gamma^m_{np} \equiv \langle \mathbf{a}^m, \nabla_{\mathbf{a}_p} \mathbf{a}_n \rangle = m\text{-component of change in } \mathbf{a}_n \text{ when evaluating}$$

$\mathbf{a}_n$  one moves from tail to tip of  $\mathbf{a}_p$ .

Here, *change in*  $\mathbf{a}_n \equiv \Delta \mathbf{a}_n = \Gamma^m_{np} \mathbf{a}_m = \nabla_{\mathbf{a}_p} \mathbf{a}_n$ . Therefore, if the basis vectors are  $\mathbf{a}_n(\rho_1)$  at lattice site  $\rho_1$ , then at an adjacent lattice site  $\rho_2$  they are

$$\mathbf{a}_n(\rho_2) = \mathbf{a}_n(\rho_1) + \Delta \mathbf{a}_n(\rho_1) = \mathbf{a}_n(\rho_1) + [\Gamma^m_{np} \mathbf{a}_m](\rho_1) = \mathbf{a}_n(\rho_1) + \nabla_{\mathbf{a}_p} \mathbf{a}_n(\rho_1).$$

In a coordinate system with constant basis vectors the covariant derivative operator is the ordinary gradient operator,  $\nabla \rightarrow {}^b\nabla$ , because the connection coefficients are all zero: *e.g.*  $\Gamma(x^a) = 0$  and  $\Gamma(X^M) = 0$  for the  $x^a$  reference frame and undeformed crystallographic coordinates  $X^M$ , respectively. It is, however, possible to express the connection coefficients for the deformed crystallographic coordinates,  $\Gamma(x^m) \equiv \Gamma^m_{np}$ , in terms of, for example, the undeformed coordinates  $X^M$

$$\Gamma^l_{MN} \equiv \lambda^L_1 (\lambda_M^m \lambda_N^n \Gamma^l_{mn} + \partial^2 x^l / \partial X^M \partial X^N),$$

or the  $x^a$  reference frame (Edelen 1962),

$$\Gamma^a_{bc} \equiv \lambda^a_1 (\lambda_b^m \lambda_c^n \Gamma^l_{mn} + \partial^2 x^l / \partial x^b \partial x^c).$$

When the 64 functions  $\Gamma^l_{mn}$  "transform" in this manner the  $x^m$  coordinates are *affinely connected*. The connection coefficients are not tensors (Misner *et al.* 1973), see also Malvern (1969).

Equivalently, **the problem** ( $g_{mn} \lambda^m \lambda^n = g_{MN}$ ) consists of solving a system of six partial differential equations in three unknowns (Truesdell and Toupin 1960):

$$g_{mn}(\partial x^m / \partial X^M)(\partial x^n / \partial X^N) = g_{MN}(X, Y, Z), \quad \text{[solution: 3 functions, } x^m = x^m(X, Y, Z) \text{]}$$

or

$$(a_m a_n \cos \theta)(\partial x^m / \partial X^M)(\partial x^n / \partial X^N) = A_M A_N \cos \theta_0,$$

where  $\mathbf{A}_M \cdot \mathbf{A}_N = A_M A_N \cos \theta_0$ . This system of equations is overdetermined, and therefore admits no solutions unless the  $g_{MN}$  satisfy integrability (or compatibility) conditions.

*"The conditions of compatibility are a necessary and sufficient condition that the space of which the continuum is a part be locally Euclidean. They are supposed to hold everywhere except possibly upon certain singular points, curves, or surfaces, where the material may divide or join. That they may fail to be satisfied upon these singular loci follows because here J becomes zero or infinite, so that for these points the first step in the theory of differential invariants cannot be taken and consequently the Riemann tensor even if it exist must fail of its usual significance. The fact that the conditions of compatibility may be meaningless or not satisfied at a junction or dislocation in a given deformation does not prevent the space in which the deformed material is embedded from being Euclidian, and consequently admissible for the later imposition of the laws of Newtonian mechanics". From Truesdell (1952).*

Components for the *Riemann curvature tensor*  $\mathbf{R}$  are (Misner *et al.* 1973)

$$R^l_{mnp} = \partial\Gamma^l_{mp}/\partial x^n + \Gamma^h_{pm}\Gamma^l_{hn} - \partial\Gamma^l_{mn}/\partial x^p - \Gamma^h_{mn}\Gamma^l_{hp}. \quad \text{DOI}$$

The completely covariant form of this tensor's components are  $R_{lmnp} = g_{lq} R^q_{mnp}$ . The vanishing of this tensor is equivalent to satisfaction of the compatibility equations (Truesdell 1952, Eshelby 1956, Nabarro 1967, Malvern 1969, Marcinkowski 1979, Kröner 1992).

Nabarro shows that for small strains  $\varepsilon_{mn} = 1/2(g_{mn} - \delta_{mn})$ ,

$$g^{mn} \approx \delta_{mn} - 2\varepsilon_{mn},$$

$$\Gamma^m_{np} \approx \varepsilon_{pm,n} + \varepsilon_{nm,p} - \varepsilon_{np,m}, \quad \text{DOI}$$

$$R^l_{mnp} \approx \partial\Gamma^l_{mp}/\partial x^n - \partial\Gamma^l_{mn}/\partial x^p, \quad [25]$$

and

$$N^{ij} = 1/4 \epsilon^{ikm} \epsilon^{jln} R_{nlmk}, \quad \text{DOI}$$

where

$$R_{nlmk} = -(\varepsilon_{mn,ik} - \varepsilon_{kn,lm} - \varepsilon_{ml,nk} + \varepsilon_{kl,nm}). \quad \text{DOI}$$

[25]: Nabarro (1967) writes  $R_{mnp}{}^l = \partial\Gamma^l_{pm}/\partial x^n + \Gamma^h_{pm}\Gamma^l_{hn} - \partial\Gamma^l_{pn}/\partial x^m - \Gamma^h_{pn}\Gamma^l_{hm}$  for the curvature tensor and  $R_{mnp}{}^l = g_{lq} R_{mnp}{}^q$  for the completely covariant components. I am following Misner *et al.* (1973); the formula for translation is  ${}^n R_{mnp}{}^l = {}^{MTW} R_{lpnm}^l$  and  ${}^n R_{mnp}{}^l = {}^{MTW} R_{lpnm}$ , *i.e.* reverse the order of the indices.

The components of  $\mathbf{R}$  can be written as  $R^{\text{lm}}_{\text{np}} = g^{\text{mq}} R^l_{\text{qnp}}$  and then contracted,  $R^{\text{lm}}_{\text{ln}} \equiv \sum_l R^{\text{lm}}_{\text{ln}} = R^{\text{m}}_{\text{n}}$ , to give the components of the *Ricci curvature tensor*  $R^{\text{m}}_{\text{n}}$  (Misner *et al.* 1973). Further contraction yields the curvature scalar,  $R$ :  $R \equiv R^{\text{m}}_{\text{m}} = R^x_x + R^y_y + R^z_z$ . As an example, for a sphere with radius  $r$ ,  $R = 2/r^2 = 2 \times \text{Gaussian curvature}$ .<sup>[26]</sup> The *Gauss-Bonnet integral* states that

$$\int_A R g^{1/2} dA = 8\pi,$$

where  $A$  is the oriented area that forms the boundary of the material. Figure 10 shows how curvature is generated from a plane-strain deformation that is incompatible:

*Incompatibility*  $\sim$  "Buckling"  $\sim$  "Curvature". 

If

$$\begin{aligned} \Gamma^{\text{m}}_{\text{np}} &= \left\{ \begin{matrix} \text{m} \\ \text{np} \end{matrix} \right\} \equiv \frac{1}{2} g^{\text{ml}} (\partial g_{\text{lp}} / \partial x^n + \partial g_{\text{ln}} / \partial x^p - \partial g_{\text{np}} / \partial x^l), \\ &= \frac{1}{2} g^{\text{ml}} (\partial \varepsilon_{\text{lp}} / \partial x^n + \partial \varepsilon_{\text{ln}} / \partial x^p - \partial \varepsilon_{\text{np}} / \partial x^l), \end{aligned}$$

with  $\left\{ \begin{matrix} \text{m} \\ \text{np} \end{matrix} \right\}$  denoting the *Christoffel symbol of the second kind*, then  $\Gamma^{\text{m}}_{\text{pn}} = \Gamma^{\text{m}}_{\text{np}} = \left\{ \begin{matrix} \text{m} \\ \text{np} \end{matrix} \right\}$ , and the solution of  $R^L_{\text{MNP}} = 0$  is

$$\Gamma^{\text{M}}_{\text{PN}} = \lambda_{\text{m}}^{\text{M}} \partial_{\text{P}} \lambda_{\text{N}}^{\text{m}},$$

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[26]: The *Gaussian curvature* for a surface with *principal radii of curvature*  $r_1$  and  $r_2$  is  $1/r_1 \times 1/r_2$  (Misner *et al.* 1973, Kreyszig 1991).

where  $\Gamma_{\text{PN}}^M$  are connection coefficients for the  $x^m$  coordinates written as functions of undeformed  $X^M$  coordinates (Kröner 1992). When  $\Gamma_{\text{NP}}^m = \Gamma_{\text{PN}}^m$ , the *torsion tensor components*

$$T_{\text{NP}}^m \equiv \Gamma_{\text{NP}}^m - \Gamma_{\text{PN}}^m,$$

or

$$\begin{aligned} T_{\text{NP}}^M &\equiv \Gamma_{\text{NP}}^M - \Gamma_{\text{PN}}^M, \\ &= \lambda_m^M (\partial_N \lambda^m_p - \partial_p \lambda^m_N), \\ &= \lambda_m^M (\partial_N \gamma_p^m - \partial_p \gamma_N^m), \end{aligned}$$

are zero, so that  $\partial_p \lambda^m_N = \partial_N \lambda^m_p$ . Here,

$$\lambda^m_N \equiv \delta^m_N + \partial_N u^m \equiv \delta^m_N + \gamma_N^m, \quad \gamma_N^m \equiv \partial u^m / \partial X^N,$$

$\gamma_N^m$  denoting components of the *elastic distortion tensor* and  $\lambda^m_N$  components for the *deformation "gradient"*. So for this zero-torsion case the surfaces of the deformed  $x^m$  coordinates,  $\vec{d}x^m$ , are level or curl-free, *i.e.* the cotangent basis vectors  $\vec{d}x^m \equiv \mathbf{a}^m$  are given by the "gradients"  $\vec{d}x^m = \lambda^m_M \vec{d}X^M$ . Therefore, exterior differentiation of the  $\mathbf{a}^m$ ,  $\vec{d}\mathbf{a}^m = \vec{d}(\vec{d}x^m) = \vec{d}^2 x^m$  produces zero, *i.e.* the Poincaré lemma:

$$\begin{aligned} \vec{d}(\vec{d}x^m) &= \vec{d}(\lambda^m_M \vec{d}X^M) = (\partial \lambda^m_M / \partial X^N) \vec{d}X^N \wedge \vec{d}X^M, \\ &= \frac{1}{2} (\partial \lambda^m_M / \partial X^N - \partial \lambda^m_N / \partial X^M) \vec{d}X^N \wedge \vec{d}X^M \equiv \partial_{[N} \lambda^m_{M]} \vec{d}X^N \wedge \vec{d}X^M, \\ &\equiv \frac{1}{2} T^m_{NM} \vec{d}X^N \wedge \vec{d}X^M = 0, \\ &\equiv -T^m. \end{aligned}$$

Here,

$$T^m \equiv T(\vec{d}x^m, \dots, \dots) \equiv \frac{1}{2} T_{NM}^m \vec{d}X^M \wedge \vec{d}X^N$$

are the torsion 2-forms, Misra (1992) also defines them like this, and  $T(\dots, \dots, \dots)$  denotes the torsion tensor. This tensor has components

$$T_{NM}^m \equiv \partial \lambda_M^m / \partial X^N - \partial \lambda_N^m / \partial X^M \equiv \partial_N \lambda_M^m - \partial_M \lambda_N^m \equiv 2 \partial_{[N} \lambda_{M]}^m,$$

which are in *mixed* form (Schouten 1989) since two different coordinate systems are used; Nabarro (1967) discusses the torsion tensor in this form. Since  $\lambda_N^m \equiv \delta_N^m + \gamma_N^m$ ,  $T_{NM}^m = \partial_N \gamma_M^m - \partial_M \gamma_N^m$ , and therefore

$$T^m = \vec{d}\tilde{\gamma}^m = \text{rot } \tilde{\gamma}^m,$$

$\tilde{\gamma}^m \equiv \gamma_N^m \vec{d}X^N$  denoting the distortion 1-forms. When  $-T^m = \vec{d}a^m = 0$  the  $a^m$  can be expressed as "gradients,"  $a^m \equiv \vec{d}x^m$ , of the coordinate functions  $x^m$ .

The connection coefficients can be written as the sum of one-half the antisymmetric part and one-half the symmetric part (Edelen 1962):

$$\Gamma_{mn}^l = \frac{1}{2}(\Gamma_{mn}^l - \Gamma_{nm}^l) + \frac{1}{2}(\Gamma_{mn}^l + \Gamma_{nm}^l) \equiv \Gamma_{[mn]}^l + \Gamma_{(mn)}^l \equiv \frac{1}{2} T_{mn}^l + \left\{ \begin{matrix} l \\ mn \end{matrix} \right\}.^{[27]}$$

[27]: Some workers (Hlavatý 1953, Schouten 1954, 1989, Edelen 1962, Kondo 1964, Nabarro 1967, Marcinkowski 1979, Kröner 1992) define components for the torsion tensor as  $T_{mn}^l \equiv \Gamma_{[mn]}^l \equiv \frac{1}{2}(\Gamma_{mn}^l - \Gamma_{nm}^l)$ . I am following Marsden and

The torsion tensor therefore measures the antisymmetric part of the connection (Nash and Sen 1983) and the Christoffel symbols measure the symmetric part; thus  $\mathbf{T} = \mathbf{0} \Rightarrow \Gamma^l_{mn} = \frac{1}{2} \{ \Gamma^l_{mn} - \Gamma^l_{nm} \}$ .

The *torsion tensor* is a function for one 1-form and one bivector (see the appendix for explanation of the index reversal):

$$\begin{aligned}
T(\dots, \dots, \dots) &\equiv T^m_{np} \mathbf{a}_m \otimes \mathbf{a}^p \otimes \mathbf{a}^n \equiv 2\Gamma^m_{[np]} \mathbf{a}_m \otimes \mathbf{a}^p \otimes \mathbf{a}^n \equiv (\Gamma^m_{np} - \Gamma^m_{pn}) \mathbf{a}_m \otimes \mathbf{a}^p \otimes \mathbf{a}^n, \\
&= \frac{1}{2} T^m_{np} \mathbf{a}_m \otimes \mathbf{a}^p \otimes \mathbf{a}^n - \frac{1}{2} T^m_{pn} \mathbf{a}_m \otimes \mathbf{a}^p \otimes \mathbf{a}^n, \quad (T^m_{np} = T^m_{[np]} \text{ is antisymmetric}) \\
&= \frac{1}{2} T^m_{np} \mathbf{a}_m \otimes \mathbf{a}^p \otimes \mathbf{a}^n - \frac{1}{2} T^m_{np} \mathbf{a}_m \otimes \mathbf{a}^n \otimes \mathbf{a}^p, \quad (\text{index exchange}) \\
&= \frac{1}{2} T^m_{np} \mathbf{a}_m \otimes (\mathbf{a}^p \otimes \mathbf{a}^n - \mathbf{a}^n \otimes \mathbf{a}^p), \\
&\equiv \frac{1}{2} T^m_{np} \mathbf{a}_m \otimes \mathbf{a}^p \wedge \mathbf{a}^n. \quad (\text{Definition of wedge product.}) \quad \square
\end{aligned}$$

A vector  $\mathbf{v}$  is *parallel transported* from point  $\rho_0$  to point  $\rho$  if its components,  $v^m$ , are the same at each point,  $v^m_0 = v^m = (v^x, v^y, v^z)$  (Misner *et al.* 1973). A *geodesic* is a parameterized curve,  $\rho(s)$ , that parallel-transports its tangent vector, say  $\mathbf{v}$ , where  $\mathbf{v} \equiv d\rho/ds$  and  $v^m = dx^m/ds$ , along itself,  $\nabla \mathbf{v} = \mathbf{0}$ . Since  $\nabla \mathbf{v} = v^m \nabla_{a_m} \mathbf{v}$ , with the covariant derivative of a contravariant vector being

$$\nabla_{a_n} \mathbf{v} \equiv \nabla \mathbf{v}(\dots, a_n) \equiv (\partial_n v^m + \Gamma^m_{pn} v^p) \mathbf{a}_m \equiv v^m_{;n} \mathbf{a}_m,$$

components of  $\nabla \mathbf{v} = v^m \nabla_{a_m} \mathbf{v} = \mathbf{0}$  give

$$\frac{d^2 x^m}{ds^2} + \Gamma^m_{np} \frac{dx^p}{ds} \frac{dx^n}{ds} = 0,$$

Hughes (1983), Nash and Sen (1983), Wald (1984), Burke (1985) and Wasserman (1992), by omitting the factor of one-half: here,  $T^l_{mn} \equiv 2\Gamma^l_{[mn]} \equiv (\Gamma^l_{mn} - \Gamma^l_{nm})$ .

the *geodesic equation*. It can be solved for the coordinates  $x^m(\rho)$  when *initial data*,  $x^m(\rho_0)$  and  $[dx^m/ds](\rho_0)$ , are provided for any given point  $\rho_0$ . The crystallographic coordinates  $x^m$  which represent *lattice lines* are examples of geodesics (Bilby 1960). The geodesic equation is governed solely by the symmetric part of the connection: any antisymmetric connection (*e.g.* dislocation density) can be added without affecting the differential equations for the lattice lines.

When  $T = \mathbf{0}$  the  $\mathbf{a}^m$  of the deformed coordinates  $x^m$  are the "gradients"  $\mathbf{a}^m = \vec{\mathbf{d}}x^m = \lambda^m_N \vec{\mathbf{d}}X^N$  (Hlavatý 1953) (with  $\lambda^m_N = \delta^m_N + \partial_N u^m \equiv \delta^m_N + \gamma_{N^m}$ ). When  $R = \mathbf{0}$  and  $T = \mathbf{0}$  the system  $g_{mn}(\partial x^m / \partial X^M)(\partial x^n / \partial X^N) = g_{MN}(X, Y, Z)$  (where  $\partial x^m / \partial X^M = \lambda^m_N$ ) is ***completely integrable*** (Hlavatý 1953). If  $T \neq \mathbf{0}$  the cotangent basis vectors  $\mathbf{a}^m$  are not gradients of the coordinates  $x^m$ ,  $\mathbf{a}^m \neq \vec{\mathbf{d}}x^m$ .

If there is no torsion, then the *divergence*,  $\mathbf{div} \equiv \nabla \bullet \equiv \nabla \bullet$ , of a contravariant tensor  $\mathbf{N} = N^{mn} \mathbf{a}_m \otimes \mathbf{a}_n$  gives a vector (Levi-Cevita 1977),

$$\nabla \bullet \mathbf{N} \equiv N^{mn}_{;m} \mathbf{a}_n \equiv \nabla \bullet \mathbf{N} \equiv N^{ab}_{,a} \mathbf{i}_b,$$

and similarly for the other index. Kröner (1992) develops an expression for **div** for the case where  $T \neq \mathbf{0}$  in order to write the Bianchi identity.

The Lie derivative and covariant derivative are used to write the torsion tensor and Riemann curvature tensor; see the appendix for a full accounting. The Lie derivative, Figure 11, is associated with the concept of "holonomy" (Burke 1985), Figure 12. "Holonomy" is related to the concept of a conservative vector field. The torsion tensor is proportional to the

dislocation density and the Riemann curvature tensor is proportional to the disclination density (Eshelby 1956, Bilby 1960, Kondo 1964, Nabarro 1967, Marcinkowski 1979); but both dislocations and disclinations have torsion  $\mathbf{T}$  and curvature  $\mathbf{R}$  (Marcinkowski 1979). The *dislocation* is defined by Figure 13 and the *disclination* by Figure 14. *Anholonomy* for an edge dislocation is shown by Figure 15.

The Lie derivative, torsion tensor, and Riemann curvature tensors are all "commutators" of vector fields. *Commutators* measure the path dependence, or non-conservative nature of vector fields. The Lie derivative measures the path dependence of two vector fields, say  $\mathbf{u} \equiv u^m \partial/\partial x^m$  and  $\mathbf{v} \equiv v^m \partial/\partial x^m$ , by taking the difference between the result of parallel transporting  $\mathbf{v}$  along  $\mathbf{u}$ ,  $\mathbf{u}[\mathbf{v}]$ , and  $\mathbf{u}$  along  $\mathbf{v}$ ,  $\mathbf{v}[\mathbf{u}]$ :

$$\text{Lie derivative of } \mathbf{v} \text{ along } \mathbf{u} \equiv \mathbf{f}_\mathbf{u}\mathbf{v} \equiv \mathbf{u}[\mathbf{v}] - \mathbf{v}[\mathbf{u}] \equiv [\mathbf{u}, \mathbf{v}],$$

where  $\mathbf{u}[\mathbf{v}]$  is the directional derivative of  $\mathbf{v}$  with respect to  $\mathbf{u}$  and  $[\mathbf{u}, \mathbf{v}]$  is the *commutator* of  $\mathbf{u}$  and  $\mathbf{v}$ . The torsion tensor does the same thing but the two vector fields are the covariant derivatives  $\nabla_\mathbf{u}\mathbf{v}$  and  $\nabla_\mathbf{v}\mathbf{u}$ , such that the path dependence of  $\nabla_\mathbf{u}\mathbf{v}$  and  $\nabla_\mathbf{v}\mathbf{u}$  is measured:

$$\text{Torsion} \equiv \mathbf{T}(\dots, \mathbf{u}, \mathbf{v}) \equiv [\nabla_\mathbf{u}, \nabla_\mathbf{v}] - [\mathbf{u}, \mathbf{v}] \equiv (\nabla_\mathbf{u}\mathbf{v} - \nabla_\mathbf{v}\mathbf{u}) - [\mathbf{u}, \mathbf{v}].$$

If  $\mathbf{T} \neq \mathbf{0}$  then the connection is *non-Riemannian*. The Riemann curvature tensor is similar but the two vector fields are "second covariant derivatives" of a vector field  $\mathbf{w}$  (which is why the term curvature is used),

$$\begin{aligned}
Riemann &\equiv \vec{d}^2 w(u, v) \equiv \mathfrak{R}(u, v)w \equiv \langle \vec{d}^2 w, u \wedge v \rangle = V_u V_v w - V_v V_u w - V_{[u,v]} w, \\
&= R(\dots, w, u, v),
\end{aligned}$$

where

$$\langle \mathfrak{R}, u \wedge v \rangle \equiv \mathfrak{R}(u, v),$$

$\mathfrak{R}$  denoting the *curvature operator*. For a *general affine connection*, Schouten (1954), Nash and Sen (1983), and Wasserman (1992) show that both the torsion and curvature tensors are required to measure the path dependence of a vector field  $v$ :

$$[V_{a_m} V_{a_n} v - V_{a_n} V_{a_m} v]^p = v^p_{,mn} - v^p_{,nm} = v^q R^p_{qnm} - v^p_{,q} T^q_{mn},$$

and as shown in the Appendix

$$\{V_u V_v - V_v V_u\}w = R(\dots, w, u, v) - T(Vw, u, v).$$

The torsion tensor vanishes for a *Riemannian connection* and, if the manifold is *flat*, then  $R = \mathbf{0}$ , and it is *Euclidian*.

*"To state physical laws in quantitative form, we are compelled to deal with vectors and tensors in curved space. These quantities are not most conveniently described in the familiar language of tensor calculus when the space is multiply connected. A new or intrinsic formulation is required.*

*Tensor analysis is not adequate. It demands a nonsingular coordinate system with respect to which one can give the components of vectors and tensors. However, according to the definition of a differentiable manifold, a single nonsingular coordinate system is not enough to cover a manifold that is topologically inequivalent to an open set in Euclidian space. It is essential for our physical applications that we be able to distinguish singular tensor fields from nonsingular ones. A singularity in a field will ordinarily imply a localized source term in the differential equations. Such a source term will represent a nongeometric charge or mass which has not been eliminated from the theory, but merely idealized to a point charge or a point mass. To investigate the content of pure geometrodynamics we therefore exclude all singularities in the fields. ... If we do not know what nonsingular coordinates are, then we have not yet defined the differentiable structure of the manifold. However, as soon as we have said what we mean by a differentiable function, then the idea of a differentiable tensor field is well defined: A tensor is differentiable at a point  $x$  if its components with respect to a (nonsingular) coordinate system around  $x$  are differentiable functions at  $x$  (Misner and Wheeler 1957).*

Differential forms (exterior calculus) provide the "intrinsic representation" for tensors (Misner and Wheeler 1957). A crystallographic coordinate "patch" containing a dislocation is singular at the dislocation core. Eliminating the core from the patch produces a doubly-connected region. The crystallographic coordinate system for the material is made by joining all "patches" together smoothly. The torsion tensor  $T$  for a continuum with defects contains the information lost from this cutting process. The dislocation torsion tensor  $T$  describes the singularity. Incompatibility,  $N \neq 0$ , is equivalent to "curvature,"  $R \neq 0$ , and if non-fitting blocks of matter are "forced" together, "buckling" results. Disclinations are "buckling defects;" see Nabarro (1967), Kröner and Anthony (1975) and, especially Venkataraman and Sahoo's (1985) Fig. 22. An edge dislocation core may also "buckle" (Nabarro 1967). Thus, for a lattice with disclinations,  $R \neq 0$  holds globally, while for a lattice with only dislocations,  $R = 0$  except at dislocation cores (Truesdell 1952, Marcinkowski 1979).

The mathematical procedure followed in the remainder of this subsection, adapted from Misner *et al.* (1973) is summarized next. It is discussed in more detail in this Chapter's Appendix. The torsion tensor is discussed further in the box which follows, and more completely in the Appendix.

Mathematical Procedure: Duality ( $\rightarrow$ ) and Differentiation ( $\downarrow$ )

$g$  (metric)



$\nabla \equiv \vec{d}$  (parallel transport, covariant derivative, "generalized covariant derivative")



$\mathfrak{R} \equiv \vec{d}^2$  (curvature operator)  $\rightarrow$   $*^b \mathbf{R}^* \equiv \tilde{\mathbf{N}}$  (defects)  $\rightarrow$   $\vec{d} \tilde{\mathbf{N}} = \mathbf{0}$   
("Bianchi identities")



$\vec{d} \mathfrak{R} = \mathbf{0}$  (THE Bianchi Identity)

All of the Bianchi identities mean that the boundary of a boundary is zero (Misner *et al.* 1973). See Figure 7c.

## Torsion

The exterior derivative  $\vec{d}$  of something that can be expressed as a "gradient," e.g.  $\vec{d}f$ , automatically vanishes in a coordinate system where the cotangent basis vectors are "gradients,"  $A^M \equiv \vec{d}X^M$ :

$$\vec{d}f = (\partial f / \partial X^M) \vec{d}X^M = \partial_M f \vec{d}X^M;$$

$$\vec{d}^2 f = \partial_N \partial_M f \vec{d}X^N \wedge \vec{d}X^M = \frac{1}{2}(\partial_N \partial_M f - \partial_M \partial_N f) \vec{d}X^N \wedge \vec{d}X^M = \mathbf{0}.$$

**The basis vectors  $A^M \equiv \vec{d}X^M$  do not contribute to the operation of exterior differentiation** (Misner and Wheeler 1957). Thus,  $\vec{d}^2 f = \mathbf{0}$  and  $\partial^2 f / \partial X^M \partial X^N = \partial^2 f / \partial X^N \partial X^M$ . This will, however, not be the case if  $\vec{d}f$  is written with some other system of basis vectors, say  $a^m \neq \vec{d}x^m$ , as  $\vec{d}f \equiv v_m a^m$  (Misner and Wheeler 1957). ( $\vec{d}^2 f = \mathbf{0}$  is analogous to the vector identity  $\nabla \times \nabla f = \mathbf{0}$  which says that the curl of any gradient is zero; gradients are level surfaces.)

A general covariant vector, say  ${}^b v = v_M \vec{d}X^M$ , need not be a "gradient:" i.e.  $v_M \neq \partial f / \partial X^M$ . Then

$$\vec{d}{}^b v = (\partial v_M / \partial X^N) \vec{d}X^N \wedge \vec{d}X^M = \frac{1}{2}(\partial v_M / \partial X^N - \partial v_N / \partial X^M) \vec{d}X^N \wedge \vec{d}X^M \equiv \text{rot } v.$$

The surfaces of the 1-form  ${}^b v$  "curl" unless  $\text{rot } v = \mathbf{0}$ : e.g. like the magnetic field (\*B) around a current carrying wire (Burke 1985). In general  $\text{rot } v \neq \mathbf{0}$ , but if  $\text{rot } v = \mathbf{0}$ , i.e.  $\frac{1}{2}(\partial v_M / \partial X^N - \partial v_N / \partial X^M) \equiv \partial_{[N} v_{M]} = 0$ , then  ${}^b v$  can be expressed as a "gradient,"

$$v_M = \partial f / \partial X^M = \partial_M f,$$

so that

$$\partial_{[N} v_{M]} = \frac{1}{2}[\partial(\partial_M f) / \partial X^N - \partial(\partial_N f) / \partial X^M] = \frac{1}{2}[\partial^2 f / \partial X^M \partial X^N - \partial^2 f / \partial X^N \partial X^M] = 0.$$

## Torsion

(Continued)

What is  $\vec{d}^2 f$  in a coordinate system where the cotangent basis vectors are not gradients,  $\mathbf{a}^m \neq \vec{d}x^m$ , but are defined in some other manner? "Gradients" can still be written as  $\vec{d}f = (\partial f / \partial x^m) \mathbf{a}^m$ , i.e. the  $\mathbf{a}^m$  are locally meaningful (Dzyaloshinskii and Volovick 1980). Then

$$\begin{aligned}\vec{d}\vec{d}f &= \vec{d}[(\partial f / \partial x^m) \mathbf{a}^m] \\ &= [\partial(\partial_m f) / \partial x^n] \mathbf{a}^n \wedge \mathbf{a}^m + \partial_m f \vec{d}\mathbf{a}^m, \\ &= \frac{1}{2}(\partial_n \partial_m f - \partial_m \partial_n f) \mathbf{a}^n \wedge \mathbf{a}^m + \partial_p f \vec{d}\mathbf{a}^p. \quad (m \rightarrow p \text{ in } \partial_m f \vec{d}\mathbf{a}^m.)\end{aligned}$$

The quantity  $\vec{d}\mathbf{a}^p$  is evaluated like this:

$$\begin{aligned}\vec{d}\mathbf{a}^p &= \vec{d}(\lambda^p_M \vec{d}X^M) = (\partial \lambda^p_M / \partial X^N) \vec{d}X^N \wedge \vec{d}X^M, \\ &= \frac{1}{2}(\partial \lambda^p_M / \partial X^N - \partial \lambda^p_N / \partial X^M) \vec{d}X^N \wedge \vec{d}X^M, \\ &= \frac{1}{2}(\partial_N \lambda^p_M - \partial_M \lambda^p_N) \vec{d}X^N \wedge \vec{d}X^M, \\ &\equiv \frac{1}{2}(\Gamma^p_{NM} - \Gamma^p_{MN}) \vec{d}X^N \wedge \vec{d}X^M, \\ &\equiv \frac{1}{2}T^p_{NM} \vec{d}X^N \wedge \vec{d}X^M, \\ &\equiv \frac{1}{2}T^p_{nm} \mathbf{a}^n \wedge \mathbf{a}^m. \quad (T^p_{nm} = \lambda^p_N \lambda^N_m T^p_{NM}).\end{aligned}$$

Therefore

$$\begin{aligned}\vec{d}\vec{d}f &= \frac{1}{2}(\partial_n \partial_m f - \partial_m \partial_n f) \mathbf{a}^n \wedge \mathbf{a}^m + \frac{1}{2}(\partial_p f) T^p_{nm} \mathbf{a}^n \wedge \mathbf{a}^m, \\ &= \mathbf{0} + \frac{1}{2}(\partial_p f) T^p_{nm} \mathbf{a}^n \wedge \mathbf{a}^m;\end{aligned}$$

a formula which Schouten (1954) lists in component form. See Choquet-Bruhat *et al.* (1982) as well. I assumed that  $\partial_n \partial_m f - \partial_m \partial_n f = 0$ ; partial differentiation commutes in a "holonomic" coordinate system (Misner *et al.* 1973).

## 2.1. Dislocations

A dislocation loop is constructed by cutting the crystal over a (close-packed) surface  $\mathbf{A}$  that is bounded by a closed curve  $\mathbf{C}$ , and then displacing the top lattice over a (close-packed) distance  $-\mathbf{b}$  while keeping the lower lattice fixed in place (de Wit 1960). The unit normal vector  $\mathbf{n}$  to  $\mathbf{S}$  is related to  $\mathbf{C}$  by the *right-hand screw rule*:  $\mathbf{n}$  is contained in the extra-half plane of the positive edge segment of the dislocation loop;  $-\mathbf{n}$  is contained in the extra-half plane of the negative edge segment. **The dislocation loop can be therefore modelled with a "dipole" of positive and negative edge dislocations** (Nabarro (1967).

Figure 16 shows a *glide type edge dislocation dipole* that has been "*nucleated*" in a perfect crystal. After the right-most dislocation glides to the surface of the crystal a single edge dislocation remains. Both the dislocation dipole and single dislocation shown here are "*quantized*" defects (Marcinkowski 1979). "*Quantized*" defects produce lower internal energy in the crystal when "*relaxed*," but they are easier to model and display. The dislocation pair of Figure 16 is very similar to *Dehlinger's Verhakung* (Nabarro 1967), which is shown by Figure 17. The edge dislocation is a "*singularity*" (Friedel 1979). A *singularity* can be defined as an incomplete geodesic (Wald 1984); a good description of an edge dislocation. An analysis of the single "*quantized*" edge dislocation of Figure 16c is presented next, following Marcinkowski's (1979) treatment to some extent. The geometry for this analysis is illustrated by Figure 18. I am following the convention for the Burgers vector given by Hirth and Lothe (1982): A positive edge dislocation has axis (core) running into the paper, the extra-half plane runs from the axis to the top of the page and the Burgers vector points to the left. See Edelen (1987) for discussion of screw dislocations.

### 2.1.1. The Dislocated State and Dislocation Strain Tensor

The dislocated state of Figure 18c is generated from the *reference state* ( $X^M$ ), Figure 18a, by inserting an *extra half-plane*, or singularity, into the  $X^M$  coordinates. This *dislocation deformation* is described with a matrix  $A^m_M$ : Recall for an elastic deformation that the cotangent basis vectors  $\mathbf{a}^m \equiv \vec{\mathbf{d}}x^m$  for the deformed coordinate system ( $x^m$ ) are  $\vec{\mathbf{d}}x^m = \lambda^m_M \vec{\mathbf{d}}X^M$ , where the matrix elements  $\lambda^m_M$  are functions of the undeformed coordinates,  $\lambda^m_M = \lambda^m_M(X^P)$ . Thus,

$$\mathbf{a}^m \equiv A^m_M \mathbf{A}^M \equiv A^m_M \vec{\mathbf{d}}X^M$$

for the *dislocation deformation*; but the  $\mathbf{a}^m$  are not equivalent to  $\vec{\mathbf{d}}x^m$ : The "dislocation torsion"  $\mathbf{T}$  produces torsion  $T$  in the crystallographic coordinates, so the  $\mathbf{a}^m$  are not "gradients" of the deformed crystallographic coordinates  $x^m$ . The dislocation of Figure 18c terminates at  $X = Y = 0 = x = y$  and its axis lies along the Z-axis (z-axis). Thus, the only non-zero components of  $A^m_M$  are

$$A_x^x = H(Y)[\delta(X) + 1] + H(-Y),$$

$$A_y^y = A_z^z = 1,$$

as shown by Figure 18d. Here,  $H(X)$  is the *Heavyside function* (Choquet-Bruhat *et al.* 1982),

$$H(X) = \{0 \text{ if } X < 0 \text{ and } 1 \text{ if } X > 0\},$$

$$H(-X) = \{0 \text{ if } X > 0 \text{ and } 1 \text{ if } X < 0\},$$

$$H(0) = \text{undefined};$$



and  $\delta(X)$  is the Dirac delta function. The *Dirac delta function* is (Morse and Feshbach 1953)

$$\delta(X) \equiv \lim_{\Delta \rightarrow 0} (1/\Delta), \text{ for } -\Delta/2 < X < \Delta/2,$$

$$\delta(X) = 1 \text{ for } X = 0,$$

$$\delta(X) = 0 \text{ for } X < -\Delta/2 \text{ or } X > \Delta/2.$$
<sup>[28]</sup>

Both the Heaviside and Dirac delta functions are "pathological".<sup>[29]</sup> **Pathological functions are not continuous or differentiable at their origin.** The fancy function for  $A_m^m$  just says that there is an extra coordinate grid at the origin for  $Y > 0$  (*i.e.* an extra half-plane).

The shaded region of Figure 18c is elastically deformed. This elastic deformation is a simple shear, Figure 18e. The tangent basis vectors for the dislocated state are, again,  $\mathbf{a}_m = \lambda_m^M \mathbf{A}_M$ . Components for the metric tensor,  $\mathbf{g} \equiv g_{mn} \mathbf{a}^m \otimes \mathbf{a}^n$ , are therefore  $g_{mn} \equiv \mathbf{a}_m \cdot \mathbf{a}_n = \lambda_m^M \lambda_n^N \mathbf{A}_M \cdot \mathbf{A}_N \equiv \lambda_m^M \lambda_n^N G_{MN}$ . The tensor can then be written as

$$\mathbf{g} \equiv g_{mn} \mathbf{a}^m \otimes \mathbf{a}^n = g_{mn} (A_m^M \vec{d}X^M) \otimes (A_n^N \vec{d}X^N) = g_{mn} A_m^M A_n^N \vec{d}X^M \otimes \vec{d}X^N,$$

since  $\mathbf{a}^m \equiv A_m^M \mathbf{A}^M \equiv A_m^M \vec{d}X^M$ . The *dislocation strain tensor* is  $\boldsymbol{\epsilon} \equiv \frac{1}{2}(\mathbf{g} - \mathbf{G})$ , with  $\mathbf{G} \equiv G_{MN} \vec{d}X^M \otimes \vec{d}X^N$ ; using the last relationship for  $\mathbf{g}$ ,

[28]: Note that the units of  $\delta(X)$  are inverse to those of  $X$  (if in fact there are any associated with  $X$ ):  $[\delta(X)] = [X]^{-1}$ . Also, for a function  $f(X)$ ,

$$\int_{-\infty}^{\infty} f(\zeta) \delta(\zeta - X) d\zeta = f(X).$$

[29]: They are related:  $dH(x)/dx = \delta(x)$  (Choquet-Bruhat *et al.* 1982).

$${}^a\boldsymbol{\epsilon} \equiv \tfrac{1}{2}(\mathbf{g} - \mathbf{G}) = \tfrac{1}{2}(g_{mn} A^m{}_M A^n{}_N - G_{MN}) \vec{d}X^M \otimes \vec{d}X^N.$$

### 2.1.2. The Burgers Vector

The Burgers vector is determined for an edge dislocation by counting 1-forms representing crystallographic planes. These planes do not "mesh" in a dislocated lattice.

The dislocation axis points in the direction defined by the right hand rule. An oriented, closed path  $\mathbf{C}(x^m)$  in the dislocated crystal becomes an open circuit  $\mathbf{C}'(X^M)$  in the reference state. Thus

$$-b^m \equiv \oint_{\mathbf{C}} \mathbf{a}^m = \int_{\mathbf{C}'} A^m{}_M \vec{d}X^M$$

are components of the Burgers vector. The Burgers vector is

$$\mathbf{b} \equiv -\left(\int_{\mathbf{C}'} A^m{}_M \vec{d}X^M\right) \mathbf{a}_m.$$

Integrating the 1-form  $\mathbf{a}^m \equiv A^m{}_M \vec{d}X^M$  around the closed contour  $\mathbf{C} = sp + pq + qr + rs$ , or open contour  $\mathbf{C}' = sp + pq + qr + rf$  for the edge dislocation of Figure 18c with

$$\mathbf{b} = f\mathbf{s},$$

i.e. the **FS/RH** convention (Hirth and Lothe 1982), gives

$$\begin{aligned}
-\bar{b}^x \equiv \oint_C \mathbf{a}^m &= \int_C A^m_M \vec{d}X^M = \int_s^p A_x^y \vec{d}Y + \int_p^q A_x^x \vec{d}X + \int_q^r A_y^x \vec{d}Y + \int_r^f A_x^x \vec{d}X, \\
&= \int_p^q A_x^x \vec{d}X + \int_r^f A_x^x \vec{d}X, \\
&= \int_p^q [\delta(X) + 1] dX + \int_r^f dX = [4 + 1] + -4 = 1.
\end{aligned}$$

The open contour  $\mathbf{C}' = sp + pq + qr + rf$  is closed by adding  $\mathbf{b} = fs$ , which is the *true Burgers vector*. The "geometric nature" of this integral is displayed by Figure 18f.

An alternative calculation of the Burgers vector is

$$-\bar{b}^x = \langle \mathbf{a}^m, {}^{\text{top}}\mathbf{v} \rangle - \langle \mathbf{a}^m, {}^{\text{bot}}\mathbf{v} \rangle = 5\langle \mathbf{a}^m, \mathbf{a}_n \rangle - 4\langle \mathbf{a}^m, \mathbf{a}_n \rangle = (5 - 4)\delta^m_n = 1,$$

where  ${}^{\text{top}}\mathbf{v} \equiv pq$  and  ${}^{\text{bot}}\mathbf{v} \equiv rs$ .

The contravariant component  $b^x$  of  $\mathbf{b}$  is dimensionless,  $b^x = -1$ ; but the physical component (Malvern 1969) is

$$b^{(x)} \equiv b^x g_{xx}^{1/2} = b^x a_x = -a_x,$$

where  $a_x$  is the magnitude of  $\mathbf{a}_x$ .

### Physical Components of Vectors

In a general (even non-orthogonal) coordinate system the *physical components* of vector  $\mathbf{v}$ , denoted  $v^m$ , are its components with respect to the unit vectors  $\mathbf{i}_m$  that are parallel to the tangent basis vectors  $\mathbf{a}_m \equiv a_m \mathbf{i}_m$  (no sum), where  $a_m \equiv (\mathbf{a}_m \cdot \mathbf{a}_m)^{1/2}$  is the magnitude, or norm of  $\mathbf{a}_m$  (Malvern 1969):

$$v^m \equiv v^m g_{mm}^{1/2} \text{ for } m = x, y, z \text{ (no sum) and, } \mathbf{v} = v^m \mathbf{i}_m \text{ (sum).}$$

#### 2.1.3. The Dislocation Torsion Tensor

If  $\partial \mathbf{S}$  represents a closed  $p$ -dimensional boundary of a  $(p + 1)$ -dimensional surface  $\mathbf{S}$ , then

$$\int_S \vec{d}\omega = \int_{\partial S} \omega$$

is Stokes' theorem, written with the  $p$ -form  $\omega$  (Misner *et al.* 1973). Components of the Burgers vector  $-b^m \equiv \oint_C \mathbf{a}^m$  can be reexpressed with Stokes' theorem as

$$-b^m \equiv \oint_C \mathbf{a}^m \rightarrow \oint_{\partial S} \mathbf{a}^m = \int_S \vec{d}\mathbf{a}^m,$$

where  $\partial \mathbf{S} \equiv \mathbf{C}$  is the closed loop in the dislocated crystal that surrounds the surface  $\mathbf{S}$  (in the  $x$ - $y$  plane of Figure 18c). The exterior derivative of the cotangent basis vector is

$$\begin{aligned}
\vec{\mathbf{d}}\mathbf{a}^m &= \vec{\mathbf{d}}(A^m_M \vec{\mathbf{d}}X^M) = (\partial A^m_M / \partial X^N) \vec{\mathbf{d}}X^N \wedge \vec{\mathbf{d}}X^M, \\
&= \tfrac{1}{2}(\partial_N A^m_M - \partial_M A^m_N) \vec{\mathbf{d}}X^N \wedge \vec{\mathbf{d}}X^M, \\
&\equiv \tfrac{1}{2}(F^m_{NM} - F^m_{MN}) \vec{\mathbf{d}}X^N \wedge \vec{\mathbf{d}}X^M, \\
&\equiv \tfrac{1}{2} T^m_{NM} \vec{\mathbf{d}}X^N \wedge \vec{\mathbf{d}}X^M, \\
&\equiv -\mathbf{T}(\mathbf{a}^m, \dots, \dots);
\end{aligned}$$

where

$$F^m_{NM} \equiv \partial A^m_M / \partial X^N, (F^L_{NM} = A_m^L F^m_{NM})$$

are connecting coefficients<sup>[30]</sup> and

$$T^m_{NM} \equiv F^m_{NM} - F^m_{MN} \equiv \partial A^m_M / \partial X^N - \partial A^m_N / \partial X^M, (T^L_{NM} = A_m^L T^m_{NM})$$

are components of the *dislocation torsion tensor*  $\mathbf{T} \equiv T^m_{NM} \mathbf{a}_m \otimes \mathbf{A}^M \otimes \mathbf{A}^N$ ,

$$\mathbf{T}(\mathbf{a}^m, \dots, \dots) \equiv \tfrac{1}{2} T^m_{NM} \mathbf{A}^M \otimes \mathbf{A}^N \equiv \tfrac{1}{2} T^m_{NM} \vec{\mathbf{d}}X^M \wedge \vec{\mathbf{d}}X^N = -\vec{\mathbf{d}}\mathbf{a}^m.$$

If  $\mathbf{T} = \mathbf{0}$ , then  $\vec{\mathbf{d}}\mathbf{a}^m = \mathbf{0} \Rightarrow \oint_c \mathbf{a}^m = 0$ . Components for the Burgers vector are

$$-b^m \equiv \oint_{\partial S} \mathbf{a}^m = \int_S \vec{\mathbf{d}}\mathbf{a}^m = \tfrac{1}{2} \int_S T^m_{NM} \vec{\mathbf{d}}X^N \wedge \vec{\mathbf{d}}X^M = \iint T^m_{NM} dX^N dX^M. [31]$$

[30]: See Schouten and Kulk (1969) and Schouten (1954) for discussion about "connecting quantities" or "connecting objects," respectively.

[31]: If, for example,  $T^m_{NM} = 1$ , then this integral is just  $S' \mathbf{a}_n$ , where  $S'$  is the area of the surface being integrated;  $\mathbf{S}'$  is perpendicular to the dislocation axis.

Symbolically,

$$\mathbf{b} = b^m \mathbf{a}_m = \left( \int_{S'} \mathbf{T}(\mathbf{a}^m, \dots, \dots) \right) \mathbf{a}_m,$$

the "slots" in  $\mathbf{T}(\mathbf{a}^m, \dots, \dots) \equiv \frac{1}{2} T_{NM}^m \vec{d}X^M \wedge \vec{d}X^N = -\vec{d}\mathbf{a}^m$  being filled by a parameterization of  $S'$ . A very simple example follows.

The only non-zero component of the torsion tensor for the edge dislocation shown by Figure 18c is

$$T_{xy}^x = \delta(X)\delta(Y),$$

since it is just a singularity at the origin (or see Marcinkowski (1979) for a derivation).

Therefore,

$$b^x = \frac{1}{2} \int_{S'} T_{xy}^x \vec{d}Y \wedge \vec{d}X = -\frac{1}{2} \int_{S'} T_{xy}^x \vec{d}X \wedge \vec{d}Y,$$

since the exterior product is antisymmetric. Thus, letting the surface  $S' \rightarrow \infty$ ,

$$b^x = - \int_{-\infty}^{\infty} \delta(X) dX \int_{-\infty}^{\infty} \delta(Y) dY = -1.$$

#### 2.1.4. Elastic Strain from the Dislocation

The lattice makes way for the dislocation (strain " $\boldsymbol{\epsilon}$ ") by producing the "anti-symmetric" elastic strain  $\boldsymbol{\epsilon}$  shown by Figure 18c. Dislocations are a source of *internal strain* (Kröner and Anthony 1975). Recall that the incompatibility tensor is  $\mathbf{N} = -\epsilon^{ikm} \epsilon^{jln} \epsilon_{mn;lk} \mathbf{a}_i \otimes \mathbf{a}_j$ ;  $\mathbf{N} = \mathbf{0}$  when there are no defects (*e.g.* dislocations or disclinations) in the lattice. The elastic strain

$\boldsymbol{\varepsilon}$  resulting from a single edge dislocation is incompatible,  $\mathbf{N}(\boldsymbol{\varepsilon}) \neq \mathbf{0}$ , and similarly  $\mathbf{N}(\langle\boldsymbol{\varepsilon}\rangle) \neq \mathbf{0}$ .

In the linear approximation however,

$$\mathbf{N}(\langle\boldsymbol{\varepsilon} + \boldsymbol{\varepsilon}\rangle) = \mathbf{N}(\langle\boldsymbol{\varepsilon}\rangle) + \mathbf{N}(\boldsymbol{\varepsilon}) = \mathbf{0}.^{[32]}$$

The sum of the dislocation and linear elastic strains is compatible (Nabarro 1967, de Wit 1981), there are no gaps or overlapping regions in the lattice. Dislocations are a *source* of incompatibility  $\mathbf{N}(\langle\boldsymbol{\varepsilon}\rangle) \neq \mathbf{0}$  and the incompatibility produces elastic strain  $\boldsymbol{\varepsilon}$  (de Wit 1981). Thus,  $\mathbf{N}(\langle\boldsymbol{\varepsilon} + \boldsymbol{\varepsilon}\rangle) = \mathbf{0}$  gives the system of partial differential equations

$$\epsilon^{ikm} \epsilon^{jln} \varepsilon_{mn;lk} = -\epsilon^{ikm} \epsilon^{jln} \langle\varepsilon\rangle_{mn;lk},$$

or equivalently,

$$(\nabla_k \nabla_l \varepsilon_{mn} - \nabla_m \nabla_n \varepsilon_{kl}) = -(\nabla_k \nabla_l \langle\varepsilon\rangle_{mn} - \nabla_m \nabla_n \langle\varepsilon\rangle_{kl}). \quad [32]$$

The notation  $\nabla_m$  means the components of  $\nabla_{a_m}$ , e.g.  $\nabla_m v_n \equiv v_{n;m} \equiv v_{n,m} - v_k \Gamma^k_{nm}$  and,  $\nabla_m v^n \equiv v^n_{;m} \equiv v^n_{,m} + v^k \Gamma^m_{km}$ . Again,  $\langle\varepsilon\rangle \equiv \frac{1}{2}(g - \mathbf{G}) = \frac{1}{2}(g_{mn} A^m_M A^n_N - G_{MN}) \vec{d}X^M \otimes \vec{d}X^N$ ,  $g_{mn} \equiv \mathbf{a}_m \bullet \mathbf{a}_n = \lambda_m^M \lambda_n^N \mathbf{A}_M \bullet \mathbf{A}_N \equiv \lambda_m^M \lambda_n^N G_{MN}$  and,  $G_{MN} \equiv \mathbf{A}_M \bullet \mathbf{A}_N$ ;  $g$  is the metric for the dislocated state and  $\mathbf{G}$  is the metric for the reference state.

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[32]: For a dislocation loop or a "uniform" dislocation distribution,  $\mathbf{N}(\langle\boldsymbol{\varepsilon}\rangle) = \mathbf{0} \Rightarrow$

$\mathbf{N}(\boldsymbol{\varepsilon}) = \mathbf{0}$  (Nabarro 1967).

**"The covariant derivative can be regarded as a derivative that in some sense remains parallel to the lattice planes"** (de Wit 1981).

Figure 18c shows that outside the dislocation core the dislocation produces elastic distortion

$$\gamma_m^M \equiv \partial u^M / \partial x^m \text{ or, } \gamma_{M^m} \equiv \partial u^m / \partial X^M,$$

in the lattice. For small elastic strains such as those which obtain at distances sufficiently far away from dislocation cores, the following results (de Wit 1981, Kröner 1981):

$$\vec{d}\gamma_p^m = \Gamma_{np}^m \vec{dx}^n \Rightarrow \Gamma_{np}^m = \partial \gamma_p^m / \partial x^n = \partial_n \gamma_p^m.$$

I have written  $\vec{d}x^n$  instead of  $a^n$  here, with the stipulation that regions free of defects are differentiable. (Also, recall that  $\Gamma_{np}^m = \lambda_m^N \partial_N \lambda_p^m$ , where  $\lambda_p^m = \delta_p^m + \gamma_p^m$ ; thus,  $\Gamma_{np}^m = \lambda_n^N \lambda_p^m \Gamma_{np}^m = \lambda_n^N \lambda_p^m \partial_N \gamma_p^m$ .) The connection coefficients are used to define covariant differentiation:

$$\Gamma_{np}^m \equiv \langle \mathbf{a}^m, \nabla_{\mathbf{a}_p} \mathbf{a}_n \rangle = -\langle \nabla_{\mathbf{a}_p} \mathbf{a}^m, \mathbf{a}_n \rangle \Rightarrow \nabla_{\mathbf{a}_p} \mathbf{a}_n = \Gamma_{np}^m \mathbf{a}_m \text{ and } \nabla_{\mathbf{a}_p} \mathbf{a}^m = -\Gamma_{np}^m \mathbf{a}^n.$$

So for small strains covariant differentiation becomes

[33]: Differentiation is allowed since the dislocation core is being excluded.

$$\nabla_{\mathbf{a}_p}^b \mathbf{u} \equiv \nabla^b \mathbf{u}(\dots, \mathbf{a}_p) \equiv [\partial u_n / \partial x^p - u_m \Gamma_{np}^m] \mathbf{a}^n \approx [\partial u_n / \partial x^p - u_m \partial_n \gamma_p^m] \mathbf{a}^n,$$

$$\nabla_{\mathbf{a}_p} \mathbf{v} \equiv \nabla \mathbf{v}(\dots, \mathbf{a}_p) \equiv [\partial v^m / \partial x^p + v^n \Gamma_{np}^m] \mathbf{a}_m \approx [\partial v^m / \partial x^p + v^n \partial_n \gamma_p^m] \mathbf{a}_m,$$

for covariant vectors (or 1-forms) and vectors, respectively. A vector  $\mathbf{v}$  (1-form  ${}^b \mathbf{u}$ ) is a function for a 1-form (vector),  $\mathbf{v}(\dots)$ ; the covariant derivative of  $\mathbf{v}$ ,  $\nabla(\mathbf{v}(\dots))$ , produces a "slot,"  $\nabla(\mathbf{v}(\dots)) = \nabla \mathbf{v}(\dots, \dots)$ , to install a *direction* for differentiation,  $\nabla_{\text{direction}} \mathbf{v} = \nabla \mathbf{v}(\dots, \text{direction})$ . For very small strains covariant differentiation reverts to ordinary differentiation: *e.g.*  $\nabla_{\mathbf{a}_m} (v^n \mathbf{a}_n) \approx (\partial v^n / \partial x^m) \mathbf{a}_n$  and,  $\nabla_{\mathbf{a}_m} (u_n \mathbf{a}^n) \approx (\partial u_n / \partial x^m) \mathbf{a}^n$ .

**The covariant derivative differs from the partial derivative because lattice planes are "curved" by an elastic deformation** (de Wit 1981).

The elastic distortion  $\gamma_m^n$  changes with position such that the *torsion T of the connection*  $\nabla$  for the lattice,

$$\mathbf{T} \equiv T_{np}^m \mathbf{a}_m \otimes \mathbf{a}^p \otimes \mathbf{a}^n \equiv (\Gamma_{np}^m - \Gamma_{pn}^m) \mathbf{a}_m \otimes \mathbf{a}^p \otimes \mathbf{a}^n \equiv \frac{1}{2} T_{np}^m \mathbf{a}_m \otimes \mathbf{a}^p \wedge \mathbf{a}^n,$$

is non-zero. Figure 18c shows how  $\vec{\mathbf{d}} \mathbf{a}^m$  changes with position because of a dislocation,  $-\vec{\mathbf{d}} \mathbf{a}^m = \mathbf{T}(\mathbf{a}^m, \dots, \dots) = \frac{1}{2} T_{np}^m \mathbf{a}^p \wedge \mathbf{a}^n \equiv \mathbf{T}^m$ .

### 2.1.5. The Dislocation Density Tensor

Dual to  $\mathbf{T}(\mathbf{a}^m, \dots, \dots) \equiv \frac{1}{2} T^m_{np} \mathbf{a}^p \wedge \mathbf{a}^n$  (or to  $\mathbf{T}(\mathbf{a}^m, \dots, \dots) \equiv \frac{1}{2} T^m_{np} \mathbf{a}^p \wedge \mathbf{a}^n$ ) is the *dislocation density tensor*,  $\rho$ :<sup>[34]</sup>

$$\begin{aligned}\rho &\equiv \frac{1}{2} \epsilon^{mpq} T^n_{pq} \mathbf{a}_m \otimes \mathbf{a}_n \equiv \rho^{mn} \mathbf{a}_m \otimes \mathbf{a}_n, \\ &= (\epsilon^{m23} T^n_{23} + \epsilon^{m31} T^n_{31} + \epsilon^{m21} T^n_{21}) \mathbf{a}_m \otimes \mathbf{a}_n, \text{ or} \\ \rho &\equiv \frac{1}{2} \epsilon^{MPQ} T^N_{PQ} \mathbf{A}_M \otimes \mathbf{A}_N \equiv \rho^{MN} \mathbf{A}_M \otimes \mathbf{A}_N; \\ &= \frac{1}{2} \epsilon^{MPQ} \lambda_n^N (\partial_p \gamma_Q^n - \partial_Q \gamma_p^n) \mathbf{A}_M \otimes \mathbf{A}_N, (T^N_{PQ} = \lambda_n^N (\partial_p \gamma_Q^n - \partial_Q \gamma_p^n)) \\ &= \frac{1}{2} \epsilon^{MPQ} (\partial_p \gamma_Q^n - \partial_Q \gamma_p^n) \mathbf{A}_M \otimes \lambda_n^N \mathbf{A}_N, ("shuffling" \lambda_n^N) \\ &= \frac{1}{2} \epsilon^{MPQ} (\partial_p \gamma_Q^n - \partial_Q \gamma_p^n) \mathbf{A}_M \otimes \mathbf{a}_n \equiv \rho^{Mn} \mathbf{A}_M \otimes \mathbf{a}_n; (\mathbf{a}_n = \lambda_n^N \mathbf{A}_N) \\ &= \frac{1}{2} \epsilon^{MPQ} [\lambda_p^p \partial_p (\lambda_q^q \gamma_q^n) - \lambda_q^q \partial_q (\lambda_p^p \gamma_p^n)] \mathbf{A}_M \otimes \mathbf{a}_n, (\partial_p = \lambda_p^p \partial_p, \gamma_Q^n = \lambda_Q^q \gamma_q^n) \\ &= \frac{1}{2} \epsilon^{MPQ} \lambda_p^p \lambda_q^q (\partial_p \gamma_q^n - \partial_q \gamma_p^n) \mathbf{A}_M \otimes \mathbf{a}_n, (\lambda_q^q \text{ is not a function of the } x^p) \\ &= \frac{1}{2} \epsilon^{MPQ} \lambda_m^m \lambda_p^p \lambda_q^q (\partial_p \gamma_q^n - \partial_q \gamma_p^n) (\lambda_m^m \mathbf{a}_m) \otimes \mathbf{a}_n, (\mathbf{A}_M = \lambda_m^m \mathbf{a}_m) \\ &= \frac{1}{2} \epsilon^{MPQ} \lambda_m^m \lambda_p^p \lambda_q^q (\partial_p \gamma_q^n - \partial_q \gamma_p^n) \mathbf{a}_m \otimes \mathbf{a}_n, ("shuffling" \lambda_m^m) \\ &= \frac{1}{2} \epsilon^{mpq} (\partial_p \gamma_q^n - \partial_q \gamma_p^n) \mathbf{a}_m \otimes \mathbf{a}_n, (\epsilon^{mpq} = \lambda_m^m \lambda_p^p \lambda_q^q \epsilon^{MPQ}) \\ &= \frac{1}{2} \epsilon^{mpq} [\partial_p (\lambda_n^N \gamma_q^n) - \partial_q (\lambda_n^N \gamma_p^n)] \mathbf{a}_m \otimes \mathbf{a}_n, (\gamma_q^n = \lambda_n^N \gamma_q^n) \\ &= \frac{1}{2} \epsilon^{mpq} (\partial_p \gamma_q^n - \partial_q \gamma_p^n) \mathbf{a}_m \otimes (\lambda_n^N \mathbf{a}_n), (\lambda_n^N \text{ is not a function of the } x^p) \\ &= \frac{1}{2} \epsilon^{mpq} (\partial_p \gamma_q^n - \partial_q \gamma_p^n) \mathbf{a}_m \otimes \mathbf{A}_N \equiv \rho^{mn} \mathbf{a}_m \otimes \mathbf{A}_N; (\mathbf{A}_N = \lambda_n^N \mathbf{a}_n) \\ &\equiv \frac{1}{2} \epsilon^{mpq} T^N_{pq} \mathbf{a}_m \otimes \mathbf{A}_N.\end{aligned}$$

[34]: The dual of the 2-form  $\mathbf{T}(\mathbf{a}^m, \dots, \dots) = \frac{1}{2} T^m_{np} \mathbf{a}^p \wedge \mathbf{a}^n$  is the 1-form

$$\begin{aligned}{}^* \mathbf{T}(\mathbf{a}^m, \dots, \dots) &\equiv \frac{1}{2} \epsilon_{qrs} g^m g^{sp} T^r_{np} \mathbf{a}^q = \frac{1}{2} \epsilon_{qrs} T^{mrs} \mathbf{a}^q = \epsilon_{xyz} T^{myz} \mathbf{a}^x + \epsilon_{yzx} T^{mzx} \mathbf{a}^y + \\ &\epsilon_{zxy} T^{mxz} \mathbf{a}^y = \Omega (T^{myz} \mathbf{a}^x + T^{mzx} \mathbf{a}^y + T^{mxz} \mathbf{a}^z). \text{ Alternatively, } {}^* \mathbf{T}(\mathbf{a}^m, \dots, \dots) \equiv \\ &\frac{1}{2} \epsilon_{qrs} g^m g^{sp} T^r_{np} \mathbf{a}^q = \frac{1}{2} \epsilon_{qrs} g^m g^{sp} T^r_{np} g^{qk} \mathbf{a}_k = \frac{1}{2} \epsilon_{qrs} g^{qk} g^m g^{sp} T^r_{np} \mathbf{a}_k = \frac{1}{2} \epsilon^{knp} T^m_{np} \mathbf{a}_k \\ &= (T^{myz} \mathbf{a}_x + T^{mzx} \mathbf{a}_y + T^{mxz} \mathbf{a}_z) / \Omega.\end{aligned}$$

The torsion  $\mathbf{T}(\mathbf{a}^n, \dots, \dots) \equiv \frac{1}{2} T_{pq}^n \mathbf{a}^q \wedge \mathbf{a}^p$  and dislocation density  $\rho \equiv \frac{1}{2} \epsilon^{mpq} T_{pq}^n \mathbf{a}_m \otimes \mathbf{a}_n$  tensors therefore have the same components, as is always the case for duals. Nabarro uses the "mixed" tensor  $\rho^{mn}$  with the order of the indices reversed,<sup>[35]</sup> and Edelen (1979) uses  $\rho^{Mn}$ . Marcinkowski (1979) also uses the "mixed" tensor  $\rho \equiv \frac{1}{2} \epsilon^{MPQ} T_{PQ}^n \mathbf{A}_M \otimes \mathbf{a}_n \equiv \rho^{Mn} \mathbf{A}_M \otimes \mathbf{a}_n$ . For the single edge dislocation of Figure 18:  $\rho = \rho^{zx} \mathbf{A}_z \otimes \mathbf{a}_x = \frac{1}{2} \epsilon^{ZXY} T_{XY}^x \mathbf{A}_Z \otimes \mathbf{a}_x = G^{-1/2} T_{XY}^x \mathbf{A}_Z \otimes \mathbf{a}_x$ ;  $\rho^{zx} = \rho(\mathbf{A}^z, \mathbf{a}^x) = G^{-1/2} T_{XY}^x = T_{XY}^x / \Omega_0 = \delta(X)\delta(Y)/\Omega_0$ , which is illustrated by Figure 18g.

The first slot, or index, of  $\rho = \rho(\dots, \dots)$ , represents the direction of the dislocation axis ( $z$  for Figure 18), and the second represents the direction of the Burgers vector:

$$\begin{aligned}
 \rho(\mathbf{a}^z, \dots) &= \rho^{zn} \mathbf{a}_n = \frac{1}{2} \epsilon^{zpq} T_{pq}^n \mathbf{a}_n = \frac{1}{2} (\epsilon^{zyx} T_{xy}^n + \epsilon^{zyx} T_{yx}^n) \mathbf{a}_n, \\
 &= \frac{1}{2} (\epsilon^{zyx} T_{xy}^n - \epsilon^{zyx} T_{yx}^n) \mathbf{a}_n, \\
 &= \frac{1}{2} \epsilon^{zyx} (T_{xy}^n - T_{yx}^n) \mathbf{a}_n, \\
 &= \frac{1}{2} \Omega^{-1} (T_{xy}^n - T_{yx}^n) \mathbf{a}_n, \\
 &= \Omega^{-1} T_{xy}^n \mathbf{a}_n.
 \end{aligned}$$

The tensor  $\rho$  written in the form  $\rho = \rho^{mn} \mathbf{a}_m \otimes \mathbf{A}_n = \epsilon^{mpq} \partial_p \gamma_q^n \mathbf{a}_m \otimes \mathbf{A}_n$  has components

[35]: That is, his equation 8.26. In the first chapter of his book however, he uses the index order that I do.

$$\begin{aligned}
\rho^{mn} &= \epsilon^{mpq} \partial_p \gamma_q^N, \\
&= \frac{1}{2} \epsilon^{mpq} \partial_p \gamma_q^N - \frac{1}{2} \epsilon^{mqp} \partial_p \gamma_q^N, (\epsilon^{mpq} = -\epsilon^{mqp}) \\
&= \frac{1}{2} \epsilon^{mpq} \partial_p \gamma_q^N - \frac{1}{2} \epsilon^{mpq} \partial_q \gamma_p^N, (\text{index exchange}) \\
&= \frac{1}{2} \epsilon^{mpq} (\partial_p \gamma_q^N - \partial_q \gamma_p^N), \\
&= \frac{1}{2} \epsilon^{mpq} T_{pq}^N, (T_{pq}^N = \partial_p \gamma_q^N - \partial_q \gamma_p^N) \\
&= \frac{1}{2} (\epsilon^{yz} T_{yz}^N + \epsilon^{zy} T_{zy}^N) + \frac{1}{2} (\epsilon^{yx} T_{zx}^N + \epsilon^{yx} T_{xz}^N) + \frac{1}{2} (\epsilon^{xy} T_{xy}^N + \epsilon^{zy} T_{yx}^N), \\
&= \epsilon^{yz} T_{yz}^N + \epsilon^{zx} T_{zx}^N + \epsilon^{xy} T_{xy}^N, (T_{pq}^N \text{ is antisymmetric}) \\
&= (T_{yz}^N, T_{zx}^N, T_{xy}^N)/\Omega. \quad ("Components" \text{ of } \epsilon^{mpq} = g^{-1/2} e^{mpq} \text{ are } g^{-1/2} = \Omega^{-1}).
\end{aligned}$$

Edelen (1979) uses the components  $\rho^{mn}$  to write the dislocation density tensor as the 2-forms,

$\tilde{\rho}^N$ :

$$\begin{aligned}
\tilde{\rho}^N &\equiv \frac{1}{2} \rho^{mn} \epsilon_{mnp} \mathbf{a}^n \wedge \mathbf{a}^p, \\
&= \frac{1}{2} (\rho^{xN} \epsilon_{xnp} \mathbf{a}^n \wedge \mathbf{a}^p + \rho^{yN} \epsilon_{ynp} \mathbf{a}^n \wedge \mathbf{a}^p + \rho^{zN} \epsilon_{znp} \mathbf{a}^n \wedge \mathbf{a}^p), \\
&= \frac{1}{2} \rho^{xN} (\epsilon_{xyz} \mathbf{a}^y \wedge \mathbf{a}^z + \epsilon_{xzy} \mathbf{a}^z \wedge \mathbf{a}^y) + \dots, \\
&= \Omega \rho^{xN} \mathbf{a}^y \wedge \mathbf{a}^z + \Omega \rho^{yN} \mathbf{a}^z \wedge \mathbf{a}^x + \Omega \rho^{zN} \mathbf{a}^x \wedge \mathbf{a}^y, \\
&\quad ("components" \text{ of } \epsilon_{mnp} \equiv g^{1/2} e_{mnp} \equiv \Omega e_{mnp} \text{ are } \Omega) \\
&= T_{yz}^N \mathbf{a}^y \wedge \mathbf{a}^z + T_{zx}^N \mathbf{a}^z \wedge \mathbf{a}^x + T_{xy}^N \mathbf{a}^x \wedge \mathbf{a}^y, \\
&\equiv -\mathbf{T}(\mathbf{A}^N, \dots, \dots). \\
(\mathbf{T}(\mathbf{A}^N, \dots, \dots)) &\equiv \frac{1}{2} T_{pq}^N \mathbf{a}^q \wedge \mathbf{a}^p.
\end{aligned}$$

The components of  $\tilde{\rho}^N$  are

$$\tilde{\rho}_{np}^N \equiv \frac{1}{2} \rho^{mn} \epsilon_{mnp} = T_{np}^N.$$

⊗

$\tilde{\rho}_{yz}^N = \Omega \rho^{xN} = T_{yz}^N$ ,  $\tilde{\rho}_{zx}^N = \Omega \rho^{yN} = T_{zx}^N$ ,  $\tilde{\rho}_{xy}^N = \Omega \rho^{zN} = T_{xy}^N$ . For the single edge dislocation of Figure 18,  $\tilde{\mathbf{p}}^x = \Omega \rho^{zx} \mathbf{a}^x \wedge \mathbf{a}^y = T_{xy}^x \mathbf{a}^x \wedge \mathbf{a}^y$ , as illustrated by Figure 18h.

If  $\mathbf{V}$  is the volume of some part of the crystal whose boundary  $\partial\mathbf{V}$  is a closed two-dimensional surface, then (Edelen 1979)

$$b^N = - \int_{\partial\mathbf{V}} \tilde{\mathbf{p}}^N.$$

Here, components of the Burgers vector in the  $X^M$  coordinates are obtained by integrating in the  $x^m$  coordinate system. Using the dislocation torsion tensor,  $\mathbf{T}(\mathbf{A}^M, \dots, \dots) = \frac{1}{2} T_{np}^M \mathbf{a}^p \otimes \mathbf{a}^n$ , for  $-\tilde{\mathbf{p}}^N$ , where for the single edge dislocation of Figure 18  $T_{np}^M = T_{xy}^x = \delta(x)\delta(y)$ ,

$$\begin{aligned} b^x &= - \int_{\partial\mathbf{V}} \tilde{\mathbf{p}}^x = - \int_{\partial\mathbf{V}} T_{xy}^x \mathbf{a}^x \wedge \mathbf{a}^y = - \iint T_{xy}^x dx dy, \\ &= - \int_{-\infty}^{\infty} \delta(x) dx \int_{-\infty}^{\infty} \delta(y) dy, \\ &= -1; \end{aligned}$$

as illustrated by Figure 18i.

#### 2.1.6. The Lie Bracket and Riemann Curvature Tensor

The Lie bracket and Riemann curvature tensor  $\mathbf{R}$  are used to measure the Burgers vector here. It is well known that a material with a dislocation or other such defect/discontinuity will have  $\mathbf{R} \neq \mathbf{0}$  at the location of the discontinuity. Marcinkowski (1979), for example, discusses the Riemann curvature tensor. The Lie bracket, on the other hand, does not appear to have received any attention in this regard.

The curve **C** considered in Figure 18j is, from start to finish,

$$\mathbf{C} \equiv -\mathbf{v}(q) + -\mathbf{u}(r) + \mathbf{v}(r) + \mathbf{u}(s) + [\mathbf{u}, \mathbf{v}],$$

obtained by parallel transporting the vectors **u** and **v** along each other. Here, the *Lie bracket*,  $[\mathbf{u}, \mathbf{v}]$ , is the same as the *Lie derivative*,  $\mathfrak{L}_{\mathbf{u}}\mathbf{v} \equiv [\mathbf{u}, \mathbf{v}]$ , and

$$[\mathbf{u}, \mathbf{v}] \equiv \mathbf{u}[\mathbf{v}] - \mathbf{v}[\mathbf{u}] \equiv \partial_{\mathbf{u}}\partial_{\mathbf{v}} - \partial_{\mathbf{v}}\partial_{\mathbf{u}} \equiv u^m \partial_m(v^n \mathbf{a}_n) - v^m \partial_m(u^n \mathbf{a}_n) \equiv (u^m v^n - v^m u^n) \mathbf{a}_n,$$

with  $\partial_{\mathbf{u}} \equiv u^m \partial_m$ . The relationship

$$\mathbf{T}(\dots, \mathbf{u}, \mathbf{v}) \equiv (\nabla_{\mathbf{u}}\mathbf{v} - \nabla_{\mathbf{v}}\mathbf{u}) - [\mathbf{u}, \mathbf{v}]$$

is derived in the appendix; since  $\nabla_{\mathbf{u}}\mathbf{v} = \nabla_{\mathbf{v}}\mathbf{u} = \mathbf{0}$  because **u** is parallel transported along **v** and vice versa, it is just

$$\mathbf{T}(\dots, \mathbf{u}, \mathbf{v}) = -[\mathbf{u}, \mathbf{v}] = \mathbf{b}. \quad \text{ qed}$$

Here, **b** is the *local Burgers vector*.

The Riemann curvature tensor **R** has components given by

$$\begin{aligned} R^m{}_{npq} &\equiv \mathbf{R}(\mathbf{a}^m, \mathbf{a}_n, \mathbf{a}_p, \mathbf{a}_q) \equiv \langle \mathbf{a}^m, \mathfrak{R}(\mathbf{a}_p, \mathbf{a}_q)\mathbf{a}_n \rangle, \\ &\equiv \langle \mathbf{a}^m, (\nabla_{\mathbf{a}_p}\nabla_{\mathbf{a}_q} - \nabla_{\mathbf{a}_q}\nabla_{\mathbf{a}_p})\mathbf{a}_n \rangle, \\ &= \langle \mathbf{a}^m, [\nabla_{\mathbf{a}_p}\{\nabla_{\mathbf{a}_q}(\mathbf{a}_n)\} - \nabla_{\mathbf{a}_q}\{\nabla_{\mathbf{a}_p}(\mathbf{a}_n)\}] \rangle, \\ &= \partial_p \Gamma^m{}_{nq} + \Gamma^k{}_{nq} \Gamma^m{}_{kp} - \partial_q \Gamma^m{}_{np} - \Gamma^k{}_{np} \Gamma^m{}_{kq}, \end{aligned}$$

since  $\Gamma_{\text{eq}}^m \equiv \langle \mathbf{a}^m(\nabla_{\mathbf{a}_q} \mathbf{a}_n) \rangle$ ; here,  $\mathfrak{R}$  denotes the *curvature operator* (Misner *et al.* 1973). The curvature tensor measures the change in a vector  $\mathbf{w}$ ,  $\Delta\mathbf{w}$ , when it is transported along the closed curve  $\mathbf{C}$ , constructed from the vector fields  $\mathbf{u}\Delta a$ ,  $\mathbf{v}\Delta b$ ,  $-[\mathbf{u}, \mathbf{v}]\Delta a\Delta b$ ,  $-\mathbf{u}\Delta a$  and  $-\mathbf{v}\Delta b$ , where  $\Delta a$  and  $\Delta b$  are parameters, by "tail to tip addition:"

$$\mathbf{C} \equiv \mathbf{u}\Delta a + \mathbf{v}\Delta b + (-[\mathbf{u}, \mathbf{v}]\Delta a\Delta b) + (-\mathbf{u}\Delta a) + (-\mathbf{v}\Delta b).$$

Then

$$\Delta\mathbf{w} \equiv -\mathbf{R}(\dots, \mathbf{w}, \mathbf{u}\Delta a, \mathbf{v}\Delta b) \equiv -\Delta a\Delta b \mathfrak{R}(\mathbf{u}, \mathbf{v})(\mathbf{w}),$$

where

$$\Delta\mathbf{w} \equiv \mathbf{w}(\text{after transport}) - \mathbf{w}(\text{before transport})$$

and,

$$\mathfrak{R}(\mathbf{u}, \mathbf{v})(\mathbf{w}) \equiv \bar{\mathbf{d}}^2 \mathbf{w}(\mathbf{u}, \mathbf{v}) \equiv \langle \bar{\mathbf{d}}^2 \mathbf{w}, \mathbf{u} \wedge \mathbf{v} \rangle = \nabla_{\mathbf{u}} \nabla_{\mathbf{v}} \mathbf{w} - \nabla_{\mathbf{v}} \nabla_{\mathbf{u}} \mathbf{w} - \nabla_{[\mathbf{u}, \mathbf{v}]} \mathbf{w}.$$

Figure 18j shows the vector  $\mathbf{w}(p) \equiv {}^r\mathbf{w}$  being parallel transported along the curve  $\mathbf{C}$ ;  $\mathbf{w}$  is unaffected by this process until it crosses the line  $x = 0$ , at which point it is reflected about  $x = 0$ ,  $\mathbf{w} = {}^r\mathbf{w} \rightarrow {}^l\mathbf{w}$ ; no further changes occur in  $\mathbf{w}$  as it completes the circuit  $\mathbf{C}$ ,  $\mathbf{w}(r) = \mathbf{w}(s) = \mathbf{w}(t) = {}^l\mathbf{w}$ . Therefore,  $\Delta\mathbf{w} \equiv {}^l\mathbf{w} - {}^r\mathbf{w} = \mathbf{b}$  (Venkataraman and Sahoo 1985). I could therefore write  $R_{xy}^x = -[\delta(x)\delta(y)]/y$ , after Marcinkowski (1979) and Eshelby (1956), and then integrate  $R_{xy}^x w^y \mathbf{a}^x \wedge \mathbf{a}^y$  around  $\mathbf{C}$  to obtain  $b^x = -1$ , if it were not for the fact that as the area of integration doubles the error increases by  $2^{3/2}$  (Misner *et al.* 1973).

## 2.2. Disclinations

If dislocations are "unevenly distributed," then there will be "gradients,"  $\vec{d}\tilde{\rho}^n$ , in the dislocation density 2-forms  $\tilde{\rho}^n \equiv \frac{1}{2}\rho^{Mn}\epsilon_{MNP}\vec{d}X^N \wedge \vec{d}X^P$ , as in Figure 14b; the dislocation density tensor  $\rho = \rho^{Mn}\mathbf{A}_M \otimes \mathbf{a}_n$  has components  $\rho^{Mn} = \epsilon^{MPQ}\partial_P\gamma_Q^n = \epsilon^{MPQ}\partial_{[P}\gamma_{Q]n} = \frac{1}{2}\epsilon^{MPQ}T^n_{PQ}$ . These "gradients" are the *disclination density 3-forms*,  $\tilde{\Theta}^n$  (Edelen 1979);

$$\tilde{\Theta}^n \equiv \tilde{\Theta}^n \epsilon \equiv \vec{d}\tilde{\rho}^n = (\partial\rho^{Mn}/\partial X^M)\epsilon,$$

where

$$\tilde{\Theta}^n \equiv \partial\rho^{Mn}/\partial X^M \equiv (\vec{\nabla} \bullet \rho) \bullet \mathbf{a}^n$$

are the "components" of  $\tilde{\Theta}^n$ :

$$\begin{aligned} \vec{d}\tilde{\rho}^n &= \vec{d}(\frac{1}{2}\rho^{Mn}\epsilon_{MNP}\vec{d}X^N \wedge \vec{d}X^P), \\ &= \frac{1}{2}(\vec{d}\rho^{Mn}) \wedge \epsilon_{MNP}\vec{d}X^N \wedge \vec{d}X^P, \\ &= \frac{1}{2}(\partial_L\rho^{Mn}\vec{d}X^L) \wedge \epsilon_{MNP}\vec{d}X^N \wedge \vec{d}X^P, \\ &= (\partial_L\rho^{Mn})\vec{d}X^L \wedge \frac{1}{2}\epsilon_{MNP}\vec{d}X^N \wedge \vec{d}X^P, \\ &= (\partial_L\rho^{Mn})\delta^L_M\epsilon, (\vec{d}X^L \wedge \frac{1}{2}\epsilon_{MNP}\vec{d}X^N \wedge \vec{d}X^P = \delta^L_M\epsilon \text{ (Edelen 1979)}) \\ &= (\partial_M\rho^{Mn})\epsilon. (\delta^L_M\partial_L = \partial_M \equiv \partial/\partial X^M.) \end{aligned}$$

From Stokes' theorem,  $\int_N \tilde{\rho}^n = \int_V \vec{d}\tilde{\rho}^n$ ,

$$\ell^n = -\int_V \vec{d}\tilde{\rho}^n$$

is the "Burgers vector" for the disclinations. Here, integration is carried out in the reference coordinates  $X^M$  to produce the "Burgers vector" in the deformed coordinates  $x^m$ .

Since there are no 4-forms in a three dimensional space, the exterior derivative of any 3-form vanishes. Thus

$$\underline{\text{Bianchi Identity}}: \tilde{d}\tilde{\Theta}^n = 0,$$

which means that disclinations form uninterrupted ("odd") lines in the lattice (Rivier 1983); it is equivalent to the prior statement  $\nabla \cdot \Theta = 0$ .

The connection coefficients are  $\Gamma_{PN}^M \equiv \lambda_m^M \partial_p \lambda_n^N$ , which can be written in the deformed coordinates as  $\Gamma_{np}^m = \partial_n \gamma_p^m$  for the small elastic strains that exist at distances sufficiently far away from defects (Kröner 1981). For small strains the Riemann curvature tensor is  $R_{mnp}^l \approx \partial \Gamma_{mp}^l / \partial x^n - \partial \Gamma_{mn}^l / \partial x^p$  (Nabarro 1967). Thus, with  $\rho^{mn} \equiv \epsilon^{mpq} \partial_p \gamma_q^n$  for  $p = \rho^{mn} \mathbf{a}_m \otimes \mathbf{a}_n$ :

$$\begin{aligned} \tilde{\Theta}^n &\approx \partial_m \rho^{mn} = \partial_m (\epsilon^{mpq} \partial_p \gamma_q^n) \approx \epsilon^{mpq} \partial_m \partial_p \gamma_q^n, \\ &= \epsilon^{mpq} \partial_m \Gamma_{pq}^n, (\Gamma_{pq}^n = \partial_p \gamma_q^n) \\ &= 1/2 (\epsilon^{mpq} \partial_m \Gamma_{pq}^n + \epsilon^{mpq} \partial_m \Gamma_{pq}^n), \\ &= 1/2 (\epsilon^{mpq} \partial_m \Gamma_{pq}^n + \epsilon^{pmq} \partial_p \Gamma_{mq}^n), \\ &= 1/2 \epsilon^{mpq} (\partial_m \Gamma_{pq}^n - \partial_p \Gamma_{mq}^n), (\epsilon^{pmq} = -\epsilon^{mpq}) \\ &\approx 1/2 \epsilon^{mpq} R_{pmq}^n, (R_{pmq}^n \approx \partial_m \Gamma_{pq}^n - \partial_p \Gamma_{mq}^n) \\ &= -1/2 \epsilon^{pmq} R_{pmq}^n, (\epsilon^{pmq} = -\epsilon^{pmq}) \\ &= -1/2 e^{pmq} R_{pmq}^n / \Omega, (\epsilon^{pmq} \equiv e^{pmq} / \Omega) \\ &= -3 R_{[pmq]}^n / \Omega. (e^{pmq} R_{pmq}^n = 3! R_{[pmq]}^n.) \end{aligned}$$

Here,

$$R^n_{[pmq]} \equiv \frac{1}{3!}(R^n_{pmq} + R^n_{mqp} + R^n_{qpm} - R^n_{pqm} - R^n_{mpq} - R^n_{qmp}).$$

Summarizing:

$$\tilde{\Theta}^n \approx \partial_m \rho^{mn} \approx \epsilon^{mpq} \partial_m \partial_p \gamma_q^n \approx \frac{1}{2} \epsilon^{mpq} \partial_m T^n_{pq} \approx \frac{1}{2} \epsilon^{mpq} R^n_{pmq} = -3R^n_{[pmq]}/\Omega. \quad \text{Eq. 1}$$

This relationship is discussed for two cases: (1) torsion-free "manifold,"  $\mathbf{T} = \mathbf{0}$ , and (2) "manifold" with torsion,  $\mathbf{T} \neq \mathbf{0}$ .

For a lattice ("manifold") that is free of torsion ( $\mathbf{T} = \mathbf{0}$ )

$$\text{First Bianchi Identity: } R^n_{[pmq]} = 0 \Rightarrow \tilde{\Theta}^n = 0,$$

is an identity (Schouten 1954). If  $\nabla \cdot \mathbf{p} = \mathbf{0}$  everywhere ("globally"), then by the *divergence theorem*,  $\int_S \mathbf{p} \cdot d\mathbf{S} = \int_V \nabla \cdot \mathbf{p} dV = 0$ , or equivalently

$$0 = \int_S \tilde{\mathbf{p}}^n = \int_V \vec{d} \tilde{\mathbf{p}}^n \equiv \int_V \tilde{\Theta}^n = -\ell^n,$$

where  $\mathbf{S}$  is the surface around the lattice volume  $\mathbf{V}$ . If the result  $\int_A \mathbf{p} \cdot d\mathbf{A} = 0$ , equivalently  $\int_A \tilde{\mathbf{p}}^n = 0$ , holds for any cross section  $\mathbf{A}$  of the lattice, then all dislocations are in the form of closed loops, and there is no macroscopic bending (Kosevich 1979); if dislocations do not form closed loops, then they must penetrate the surface of the lattice.

If the "manifold" has torsion ( $T \neq 0$ ), then (Schouten 1954):

**First Bianchi Identity**

$$R^n_{[pmq]} = \nabla_m T^n_{pq] - T^k_{[qm} T^n_{p]k}}.$$

Rivier (1983) interprets these relationships between curvature and torsion tensor components and torsion "gradients" as meaning that disclination lines can terminate inside the lattice if they do so on dislocations. The equation  $R^n_{[pmq]} = \nabla_m T^n_{pq] - T^k_{[qm} T^n_{p]k}}$  is not restricted by a linear approximation.

## Schouten

Schouten's (1954) book is often cited by, for example, de Wit, Edelen, Nabarro, and Kröner. Schouten (1954, 1989) defines the connection coefficients like

$${}^s\Gamma_{ap}^m \equiv \langle \mathbf{a}^m, \nabla_{a_p} \mathbf{a}_p \rangle = -\langle \nabla_{a_p} \mathbf{a}^m, \mathbf{a}_p \rangle,$$

which is opposite in the lower indices to the way that Misner *et al.* (1973) do: *i.e.*  ${}^s\Gamma_{np}^m$   
 $\equiv {}^{MTW}\Gamma_{pn}^m$ ;  ${}^s\Gamma_{... differentiating index ...}^m \equiv {}^{MTW}\Gamma_{... differentiating index ...}^m$ . Thus, Schouten's covariant derivatives look like  $\nabla_m v_n \equiv v_{n;m} \equiv v_{n,m} - v_k \Gamma_{mn}^k$  and,  $\nabla_m v^n \equiv v_{;m}^n \equiv v_{,m}^n + v^k \Gamma_{mk}^n$ , where  $\Gamma_{np}^m = {}^s\Gamma_{np}^m$  in these formulas. Schouten defines the torsion tensor components as

$${}^sT_{np}^m \equiv \frac{1}{2}(\Gamma_{np}^m - \Gamma_{pn}^m),$$

and the Riemann curvature tensor components as

$${}^sR_{nmkl}^r \equiv 2\partial_{[n}\Gamma_{ml]}^k + 2\Gamma_{[n|r}^k\Gamma_{ml]}^r = \partial_n\Gamma_{ml}^k - \partial_m\Gamma_{nl}^k + \Gamma_{nr}^k\Gamma_{ml}^r - \Gamma_{mr}^k\Gamma_{nl}^r,$$

where  $\Gamma_{np}^m = {}^s\Gamma_{np}^m$  in both of these formulas. Schouten also writes

$$\nabla_{[n} \nabla_{m]} v^k = \frac{1}{2}R_{nmkl}^r v^l - T_{nm}^r \nabla_r v^k,$$

where  $2\nabla_{[n} \nabla_{m]} v^k \equiv \nabla_n \nabla_m v^k - \nabla_m \nabla_n v^k \equiv v_{,mn}^k - v_{,nm}^k$ . So my torsion relates to Schouten's as  $T_{mn}^r = 2{}^sT_{nm}^r$ ; and for the Riemann curvature tensor,  ${}^{MTW}R_{lmn}^k = {}^sR_{nmkl}^r$ .

### Odd-Lines

Cellular arrays are utilized in condensed matter physics to model amorphous materials. For example, vertices and edges of the lattice graph for a covalent glass are atoms and bonds, respectively (Rivier 1987).

Odd-lines (Rivier 1979), or  $2\pi$ -disclinations, govern the physical properties of glasses when modelled as an elastic continuum (Rivier 1987). *Odd-lines* are "threads" through odd-sided rings in a continuous random network, which avoid even-numbered rings, and form either closed loops or terminate at the surface of the material. *Fivefold* and *sevenfold* rings are "local centers" of positive and negative curvature, respectively, in a network of *sixfold* rings (Kléman 1985, Venkataraman and Sahoo 1985); *i.e.* the Gauss-Bonnet theorem (Rivier 1987). The former defect is a  $\Omega = \pi/3$  wedge disclination and the latter is a  $\Omega = -\pi/3$  wedge disclination,  $\Omega$  denoting the rotation vector (Kléman 1985). If these defects are adjacent, then the odd-line through them is in a "hairpin" configuration and the elastic energy (Venkataraman and Sahoo 1986) is minimized. Such a configuration results in the formation of a topological, or cellular dislocation (Morral and Ashby 1974), or disclination anti-disclination pair (Rivier 1979). These dislocations have been observed in the bubble domains of a ferromagnetic garnet (Kléman 1985) and in the columnar phase of discotic liquid crystals (Chandrasekhar and Ranganath 1986).

### 2.3. Integrability Conditions

**The crystallographic connection is completely integrable only for the case where there are no dislocations or disclinations in the lattice.**

For a manifold with both torsion and curvature the only *integrability conditions* are the following relationships between the torsion and Riemann curvature tensor components, *Bianchi's identities* (Schouten 1954):

#### Bianchi's Identities

$$\nabla_{[k} R^m_{|n|pq]} = T^r_{[pk} R^m_{|n|q]r}.$$

For the case where there is no torsion ( $T = 0$ ), they are equivalent to

$$\vec{d}\mathfrak{R} = 0,$$

where the curvature operator  $\mathfrak{R}$  is (Misner *et al.* 1973)

$$\mathfrak{R} \equiv \mathfrak{R}_m^q \mathbf{a}_q \otimes \mathbf{a}^m,$$

with

$$\mathfrak{R}_m^q \equiv \Gamma_{nr}^q \mathbf{a}^r \wedge \Gamma_{mp}^n \mathbf{a}^p + \vec{d}(\Gamma_{mp}^q \mathbf{a}^p)$$

being the *curvature 2-forms*, and

$$R^m_{\ npq} \equiv \mathbf{R}(\mathbf{a}^m, \mathbf{a}_n, \mathbf{a}_p, \mathbf{a}_q) \equiv \langle \mathbf{a}^m, \mathfrak{R}(\mathbf{a}_p, \mathbf{a}_q) \mathbf{a}_n \rangle$$

the components of the Riemann curvature tensor.

In a three dimensional space the Riemann curvature tensor can be completely expressed as a symmetric tensor (McConnell 1957):

$$\begin{aligned} {}^*\mathbf{R}^* &= \frac{1}{4}\epsilon^{rmn}\epsilon^{spq}R_{mnpq}\mathbf{e}_r \otimes \mathbf{e}_s \equiv N^s\mathbf{e}_r \otimes \mathbf{e}_s \equiv \mathbf{N}, \\ &= N^s\mathbf{e}_r \otimes \mathbf{e}_s; \end{aligned}$$

$\mathbf{N}$  is the incompatibility tensor (Nabarro 1967). Kröner (1992) uses the 1-form  $\tilde{\mathbf{N}}$ ,

$$\tilde{\mathbf{N}} \equiv \tilde{N}_m \mathbf{a}^m, \quad \tilde{N}_m \equiv \frac{1}{2}\epsilon_{mnp}N^{np},$$

along with  $\rho^{mn} = \frac{1}{2}\epsilon^{mpq}T^n_{pq}$  to write

$$\text{First Bianchi Identity: } \underset{r}{\text{div}} \rho = -\tilde{\mathbf{N}},$$

$$\text{Second Bianchi Identity: } \underset{r}{\text{div}} \mathbf{N} = 0,$$

where

$$\underset{r}{\text{div}}_m \equiv \nabla_m + T^q_{mq}$$

defines the *divergence operator in a space with torsion*,  $\underset{r}{\text{div}}$ . This operator is a replacement for the operation  $\nabla \bullet$ ,  $\nabla$  denoting the covariant derivative operator.